Eur. Phys. J. B **50**, 69–72 (2006)
DOI: 10.1140/epjb/e2006-00061-9

THE EUROPEAN
PHYSICAL JOURNAL B

The Topological Nonconnectivity Threshold and magnetic phase transitions in classical anisotropic long-range interacting spin systems

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Received 10 November 2005 / Received in final form 1st December 2005
Published online 20 February 2006 –

Abstract. We review, with emphasis on the dynamical point of view, the classical characteristics of the Topological Nonconnectivity Threshold (TNT), recently introduced in F. Borgonovi, G.L. Celardo, M. Maianti and E. Pedersoli, J. Stat. Phys. **116**, 1435 (2004). This shows interesting connections among Topology, Dynamics, and Thermo-Statistics of ferro/paramagnetic phase transition in classical spin systems, due to the combined effect of anisotropy and long-range interactions.

PACS. 05.45.-a Nonlinear dynamics and nonlinear dynamical systems – 05.45.Pq Numerical simulations of chaotic systems – 75.10.Hk Classical spin models

1 Introduction

The magnetic properties of materials are usually described in terms of system models, such as Heisenberg or Ising models where rigorous results, or suitable mean field approximations are available in the thermodynamical limit. On the other side, modern applications require to deal with nano-sized magnetic materials, whose intrinsic features lead, from one side to the emergence of quantum phenomena [1], and to the other to the question of applicability of statistical mechanics. Indeed, few particle systems do not usually fit in the class of systems where the powerful tools of statistical mechanics can be applied at glance. In particular, an exhaustive theory able to fill the gap between the description of 2 and 10^{23} interacting particles is still missing. In a similar way, long-range interacting systems belong to the class where standard statistical mechanics cannot be applied *tout court*. Indeed, they display a number of bizarre behaviors, to quote but a few, negative specific heat [2] and hence ensemble inequivalence [3], temperature jumps, and long-time relaxation (quasi-stationary states) [4]. Therefore, from this point of view, few-body short-range interacting systems share some similarities with many-body long-range ones.

Within such a scenario, and thanks to the modern computer capabilities, it is quite natural to take a different point of view, starting investigations directly from the dynamics, classical and quantum as well [5–7]. It was in this spirit that quite recently in a class of anisotropic Heisenberg-like spin lattice systems, a topological nonconnection of the phase space was discovered [6]. Initially, for historical reasons [8], this was referred to as broken ergodicity, since if the phase space is decomposable into two topologically non-connected components then a breaking of ergodicity is indeed a trivial consequence [9]. Here we prefer to call Topological Nonconnectivity Threshold (TNT) the value E_{tnt} where such a disconnection sets in upon lowering the total energy E of the system. This result was found, first numerically and later analytically, in a class of spin models where important and rigorous results have been obtained during the last century, though generally only in the thermodynamical limit. Nevertheless, to the best of our knowledge, apparently nobody took care of the dynamics, and consequently nobody spoke of this simple but relevant property.

This dynamical point of view has a few interesting classical consequences. First of all it explains, from the point of view of microscopic dynamics, the possibility of ferromagnetic behavior in small system. Indeed, in absence of external field and external noise (temperature) a magnetized system, (belonging to one component of the non-connected phase space) remains magnetized simply because it cannot move to the other component. Furthermore, our TNT is surely related to recent results [10,11] connecting topological transitions (TT) and thermo-statistical phase transitions (PT), even if such investigations again concern the thermodynamical limit only, and they relate to usual PT of canonical thermostatistics. However, it has been recently stressed [12] that microcanonical thermo-statistics is the theoretically more suitable description for systems with small size and/or long-range interactions.

In Section 2 a short description of our class of models and the topological properties of the TNT for

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finite and infinite N, pointing out the crucial role played by the XY anisotropy is given. The deep connection with long-range interaction is also reviewed. Dynamical properties and their relations with thermostatistical properties, namely the occurrence of a standard (paramagnetic/ferromagnetic) PT, using techniques from large deviation theory [14] within the microcanonical description of the system are described in Section 3. Conclusions are given in Section 4. Here we restrict to the classical case; for a recent discussion of quantum effects, we refer to [7].

2 Mechanics and topology

As a paradigmatic model example of TNT, let us consider the following class of lattice spin models, described by the Heisenberg-like Hamiltonian:

$$H = \frac{\eta}{2}\sum_{i\neq j}^{N}\frac{S_i^x S_j^x}{r_{ij}^{\alpha}} - \frac{1}{2}\sum_{i\neq j}^{N}\frac{S_i^y S_j^y}{r_{ij}^{\alpha}} \tag{1}$$

where S_i^x, S_i^y, S_i^z are the spin components, assumed to vary continuously; $i, j = 1, ...N$ label the spins positions on a suitable lattice of spatial dimension d, and r_{ij} is the inter-spin spatial separation. Here for simplicity we consider a $d = 1$ lattice. (See [15] for extensions to $d = 2, 3$.) Each spin satisfies $|\boldsymbol{S}| = 1$. Also, $\alpha \geq 0$ parametrizes the range of interactions (decreasing range for increasing α) and $-1 < \eta \leq 1$ parametrizes the XY anisotropy. For $\alpha = \infty$ we recover nearest-neighbor interactions, while $\alpha = 0$ corresponds to infinite-range interactions. A mean-field model is obtained by setting $\alpha = 0$ and including as well the (non-physical) self-interaction pairs $i = j$:

$$H_{mf} = \frac{\eta}{2}N^2(m_x)^2 - \frac{1}{2}N^2(m_y)^2, \tag{2}$$

where $m_{x,y,z} = (1/N)\sum_i^N S_i^{x,y,z}$. While this might be thought of as a negligible modification for $N \to \infty$, nevertheless it has non-negligible effects concerning the chaoticity properties of the system. Indeed, the dynamics of the mean-field system turns out to be exactly integrable [13]. Here we are not interested in the most general spin Hamiltonian giving rise to a TNT (for instance in [6,13] a term containing a transversal magnetic field B_z has been added to H). Rather, we focus on the very simple Hamiltonian (1) which already contains the two essential ingredients which give rise to the TNT, i.e. anisotropy and long-range.

Since $-1 < \eta \leq 1$ the minimum energy configuration, with energy E_{min}, is attained when all spins are aligned along the Y axis [15], which defines implicitly the easy axis of magnetization. In the same way, let us define the TNT energy E_{tnt} as the minimum energy compatible with the constraint of zero magnetization along the easy axis of magnetization:

$$E_{tnt} = Min\ [\ H\ \mid m_y = 0\ ]. \tag{3}$$

By definition, in general $E_{min} \leq E_{tnt}$, and in particular it may be that $E_{min} \neq E_{tnt}$. We call this situation topological non-connection, and, as will become clear in a moment, its physical (dynamical as well as statistical) consequences are rather interesting. Indeed, consider a system prepared at time $t = 0$ with a definite sign of magnetization, say $m_y > 0$ and an energy value $E_{min} \leq E \leq E_{tnt}$. As time goes by, the system evolves upon the constant energy surface $H(\boldsymbol{S}^N) = E$ in configuration space. Nevertheless, due to the continuity of the dynamical equations of motion the magnetization $m_y(t)$ (not a constant of motion) may well change its size, but it can never change its sign, instead. Indeed, in order to assume a value $m_y < 0$ it should have to go through at least one configuration with $m_y = 0$, which by definition cannot belong to the $E < E_{tnt}$ surface. The whole situation can be summarized as follows.

Topology: in configuration space the surface at fixed energy E is topologically non-connected in two components, each characterized by a magnetization either $m_y < 0$ or $m_y > 0$.

Dynamics: though the two components are energetically accessible on equal grounds, the ergodicity of the constant E surface is trivially broken, since there exist no dynamically allowed path in between them.

Thermo-Statistics: de-magnetization is in principle impossible below the TNT, so we may speak in some sense of a ferromagnetic phase. Of course, the application of a magnetic field, or a thermal noise, can give the energy necessary to overcome the energy barrier, thus in principle allowing for a magnetic reversal. On the contrary, for energy values $E > E_{tnt}$, de-magnetization is in principle possible, and we may speak in some sense of a paramagnetic phase. However, being above the TNT does not automatically guarantee that, for any combination of parameter values and initial conditions, a system initially magnetized at an initial time will for sure eventually demagnetize within a given finite observational time τ_{obs}. As reported in [13], two distinct dynamical regimes may come into play here. First, a quasi-integrable regime can prevent the motion from covering the whole energy surface. We can therefore say that strong chaos is somehow another necessary ingredient in order for the system to be in its paramagnetic phase. Second, even given strong enough chaoticity to "encourage" the system to explore all the available phase space, yet the system could be given not enough time to actually do it, so effectively "freezing" it within the m_y component where it started from.

For finite N systems the XY anisotropy is the only necessary ingredient in order to have $E_{tnt} > E_{min}$ and hence the TNT. For $N \to \infty$, one quickly realizes that both $E_{min} \to -\infty$ and $E_{tnt} \to -\infty$, but may still wonder whether $E_{tnt} \to E_{min}$ as well, thus making the TNT physically irrelevant. So we define the topological non-connection ratio:

$$r = \frac{E_{tnt} - E_{min}}{|E_{min}|}, \tag{4}$$

which expresses how large a fraction of the energy range is topologically non-connected. Correspondingly, we will refer to a system as topologically non-connected if $r \to$ const. $\neq 0$ in the limit $N \to \infty$.

Extensive numerical simulations using constrained optimization and analytical estimates as well have been performed in [15], in order to evaluate r.

Such results can be summarized as follows:

i) Short Range case, $\alpha > d$: it has been proved analytically that, $\forall d$ and $\eta \neq -1$, $r \to 0$ for $N \to \infty$.
ii) Long Range case, $\alpha < d$: with the aid of numerical simulations it has been proved that, for $d = 1, 2, 3$ and $\eta \neq -1$, $r \to$ const. $\neq 0$ for $N \to \infty$.

We can thus say that while the exchange anisotropy of the coupling is the only necessary ingredient to induce the presence of the TNT, in the large N limit, only long range interacting systems give rise to a non zero topological nonconnection ratio r.

3 Dynamics and thermo-statistics

Following [13] here we focus on the time evolution of the magnetization $m_y(t)$ started with some E and $m_y(0)$. Complementary, we look at its statistical distribution $P_{ens}(E, m_y)$, built via a random sampling of an ensemble of initial conditions, all with the same E. The study of $P_{ens}(E, m_y)$ will lead to another energy threshold, E_{stat}, where the system undergoes a continuous ferro/paramagnetic PT in the thermodynamical limit. Our aim is to show the connection between Dynamics and Thermo-Statistics and the relevance of E_{tnt} w.r.t. the statistical phase transtion, E_{stat}.

As usual, starting from the Hamiltonian (1) we straightforwardly derive the equations of motion:

$$\frac{d\boldsymbol{S}_i}{dt} = \{H, \boldsymbol{S}_i\}, \tag{5}$$

where $\{,\}$ are the canonical Poisson brackets. As is well-known, for such dynamical equations the total energy E and the spin moduli, $|\boldsymbol{S}_i|^2 = 1$, are constants of the motion. Usually, for energies E not too close to E_{min}, the dynamics is characterized by a positive largest Lyapunov exponent, corresponding to strongly chaotic motion [6]. Typical examples of evolution curves of $m_y(t)$ and the corresponding $P_{ens}(E, m_y)$, are shown in Figure 1. Again, the whole situation can be summarized as follows.

Thermo-Statistics: For $E < E_{tnt}$ (Fig. 1d) the two peaks of the distribution $P_{ens}(E, m_y)$ are well separated, while for $E > E_{tnt}$ (Fig. 1e) they are connected. At E_{stat} they merge into one single peak (Fig. 1f).

Restricting attention to the mean field Hamiltonian (2), a detailed statistical analysis, using techniques from large deviations theory, leads to definite predictions (see [13] for details) concerning the microcanonical (i.e., purely state-counting at fixed E) probability distribution $P_{stat}(m_y, E)$, the topological energy threshold E_{tnt}, and the thermo-statistical energy threshold E_{stat}.

Dynamics: at low energy, (Fig. 1a), the system is always magnetized, and at high energy, (Fig. 1c), the system is on average non-magnetized. In between (Fig. 1b), in the presence of strong chaos (dependent on the parameters N and E) the magnetic reversals occur completely at random, with jumping times following a Poisson distribution. Indeed the magnetization jumps erratically up and down. We can usefully define a magnetic-reversal time-scale [13], as the average time necessary to magnetization to reverse its sign.

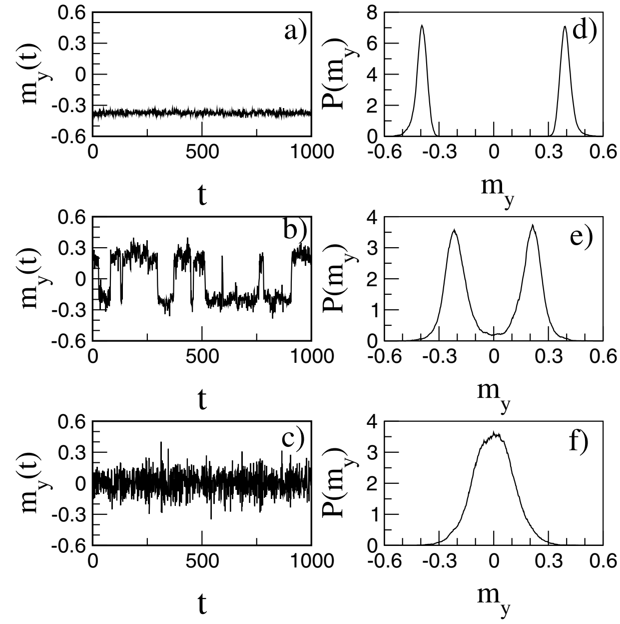

Fig. 1. Left column (a, b, c): time evolution of the magnetization $m_y(t)$ for different specific energy values. Right column (d, e, f): probability distribution of the magnetization at a given specific energy. Parameters are $\alpha = 0$, $\eta = 1$, $N = 10$. For these parameters $E_{tnt} = -0.5$ and $E_{stat} = 0$. Upper line ((a, d) below the TNT): $E/N = -0.7$. Middle line ((b, e) between the TNT and the statistical thresholds. Lower line ((c, f) above the statistical threshold) $E/N = 0.1$.

Interestingly, and somewhat reminiscent of a critical PT, as shown in Figure 2 the magnetic-reversal time-scale diverges as a power law of E at the critical energy E_{tnt}:

$$\tau_{rev} \sim \left[\frac{E - E_{tnt}}{N}\right]^{-\gamma(N)}. \tag{6}$$

Let us remark that detailed statistical consideration on the mean field model (2) lead to the analytical estimate $\gamma(N) = N$ to be compared with the numerical result $\gamma(N) \approx 0.88N$, for $\alpha = 0$ [13]. Note also that, to a rather good accuracy [13], there holds the following proportionality between the *dynamical* quantity τ_{rev} and the *statistical* quantity $P_{ens}(E, m_y)$:

$$\tau_{rev} \propto \frac{P_{max}}{P_0} \tag{7}$$

where P_{max} is the maximum value of the probability distribution and $P_0 = P_{ens}(E, 0)$.

This behavior of the magnetic-reversal time-scale has interesting consequences. Indeed adopting a viewpoint as close as possible to the experimental one, we can introduce

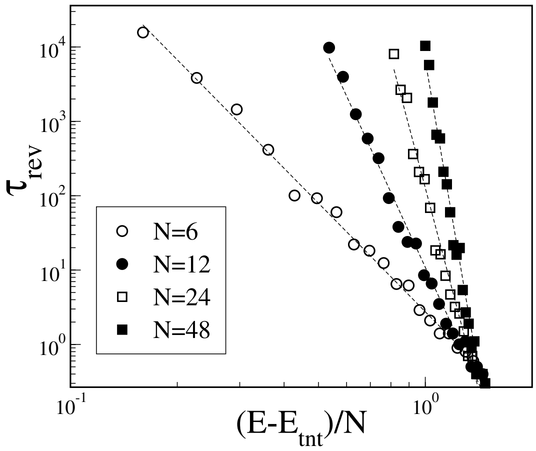

Fig. 2. Divergence of magnetization reversal times close to the TNT. Here is $\alpha = 0$, $\eta = 1$, and different N values as indicated in the insert. Lines are the best fit according to equation (6).

an observational time τ_{obs}, during which the experiment can be performed. Assuming the experimentally measured value and the dynamical time-average to coincide, we introduce the τ_{obs}-averaged magnetization: $\langle m_y \rangle_{obs} = \int_0^{\tau_{obs}} dt\, m_y(t)$. It is clear that if $\tau_{obs} \gg \tau_{rev}$ then the magnetization has time to flip between the two opposite components and, as a consequence, $\langle m_y \rangle_{obs} \simeq 0$. On the contrary, if $\tau_{obs} \ll \tau_{rev}$ the magnetization keeps its sign and cannot vanish during τ_{obs}. Defining an effective transition energy E_{obs} from the condition $\tau_{obs} = \tau_{rev}(E_{obs})$, one gets, inverting equation (6), the value of the energy at which the system is not magnetized anymore [13]. This simple argument shows the relevance of E_{tnt}, besides E_{stat}, to determine whether a system has a paramagnetic of a ferromagnetic behavior. In particular the influence of E_{tnt} on the ferromagnetic behavior of a system should be stronger in small chaotic systems where the condition $\tau_{rev} \ll \tau_{obs}$ can be expected to hold below E_{stat}.

4 Conclusions

We showed the existence in classical Heisenberg spin models of a Topological Nonconnectivity Threshold (TNT), caused by the anisotropy of the coupling when it induces an easy-axis of the magnetization. Below the TNT the constant energy surface is topologically disconnected in two components.

This result on the Topology has deep connections with the Dynamics (time-scales) and with the Thermo-Statistics (PT) of the system as well. In each component the magnetization along the easy axis has a definite sign corresponding to a ferromagnetic behavior of the system. Above the TNT, in a strong chaotic regime, the magnetization randomly reverses its sign with a characteristic time-scale which diverges as a power law at the TNT. Therefore paramagnetic behavior occurs, provided enough chaos and sufficiently large time. The connection between the TNT and the range of the interaction has also been shown. For macroscopic spin systems the existence of this threshold determines a disconnected energy range that remains relevant (w.r.t. the total energy range) for long-range interactions, while it goes to zero for short-range interactions.

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