Quasi-stationary-state duration in d -dimensional long-range model

Antonio Rodríguez¹, Fernando D. Nobre², and Constantino Tsallis^{2,3,4}

¹*GISC, Departamento de Matemática Aplicada a la Ingeniería Aeroespacial, Universidad Politécnica de Madrid, Plaza Cardenal Cisneros s/n, 28040 Madrid, Spain*

²*Centro Brasileiro de Pesquisas Físicas and National Institute of Science and Technology for Complex Systems, Rua Dr. Xavier Sigaud 150, 22290-180, Rio de Janeiro, Brazil*

³*Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, New Mexico 87501, USA*

⁴*Complexity Science Hub Vienna, Josefstädter Strasse 39, 1080 Vienna, Austria*

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Through first-principles molecular dynamics we study a d -dimensional classical inertial Heisenberg model with a range interaction decaying with distance r_{ij} as $1/r_{ij}^\alpha$ ($\alpha \geq 0$); $\alpha = 0$ ($\alpha \rightarrow \infty$) corresponds to infinite-range (nearest-neighbor) interactions; the ratio $\alpha/d > 1$ ($0 \leq \alpha/d \leq 1$) characterizes the short-range (long-range) interactions regime. In the long-range regime, a quasi-stationary state (QSS), characterized by a temperature T_{QSS} , emerges before a crossover to a second plateau, corresponding to the Boltzmann-Gibbs (BG) temperature T_{BG} (as predicted within the BG theory). The QSS duration t_{QSS} depends on the system size N , α , and d : the dependence on α appears only through the ratio α/d , and t_{QSS} decreases (increases) with α/d (with N and d). It has been possible, for fixed energy per particle, to analytically scale all these dependencies through a universal form; namely, $t_{\text{QSS}} \propto N^{A(\alpha/d)} e^{-B(N)(\alpha/d)^2}$. This paves the way for other long-range Hamiltonian systems, such as gravitation, the α -XY, and Coulombian models, among others.

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I. INTRODUCTION

Classical spin models have been largely studied due to the fact that they provide good qualitative agreement with experiments on properties of magnetic materials [1,2]. Although many studies restricted themselves to the case of nearest neighbor interactions, the introduction in 1995 of the so-called Hamiltonian mean-field (HMF) model [3], consisting in fully coupled planar rotators, including a kinetic term which enables equations of motion to be derived, opened the door to many anomalous properties (negative specific heat, quasi-stationary states, non-Maxwellian velocity probability distributions, anomalous diffusion and ergodicity breaking) thoroughly studied since then [4–11]. Those features, due to the long-range nature of the interactions, can be appropriately described within the nonextensive statistical mechanics framework (see Ref. [12] for an introduction), a current generalization of Boltzmann-Gibbs (BG) statistical mechanics, specially suited to deal with out-of-equilibrium systems in the presence of long-range correlations, based on a generalized entropy S_q [13].

This inertial ferromagnetic XY model was further generalized to the so-called α -XY model [14] via the introduction of an interaction term decaying with distance as $r^{-\alpha}$, where $\alpha \geq 0$ controls the range of the interaction, $\alpha = 0$ and $\alpha \rightarrow \infty$

corresponding respectively to the HMF and nearest-neighbor models. The α -XY model has been largely studied [15–19]. In particular, for a d -dimensional lattice, it was shown [17] that, in the high-energy regime, the largest Lyapunov exponent scales with the number N of rotators as $N^{-\kappa}$, where κ depends on (α, d) through the ratio α/d ; $\kappa > 0$ in the long-range regime ($0 \leq \alpha/d < 1$) and $\kappa \rightarrow 0$ (thus yielding positive Lyapunov exponents) in the short-range regime ($\alpha/d > 1$). In addition, q -Gaussian probability distributions (distributions that optimize the entropy S_q and generalize the Gaussian distributions in the BG theory) have been obtained for the time-averaged momenta probability distributions, both before and after the transition to the long-standing state whose kinetic temperature coincides with that of the BG equilibrium state, with a value of the entropic index $q = q_p(\alpha/d)$ within the long-range regime [19]. In contrast, the usual Maxwellian distributions are found in the short-range regime, as well as for the ensemble-averaged momenta probability distributions. Non-BG predictions are also observed for the time-averaged energy probability distributions: instead of the celebrated BG exponential, q -exponential probability distributions emerge in first-principle dynamical simulations in the long-range regime, with $q = q_E(\alpha/d)$ [19].

We may consider three-dimensional, instead of planar, rotators to get classical inertial ferromagnetic Heisenberg models [20–24], less studied in the literature. Beyond the nearest-neighbor case [20], the fully coupled model (infinite range interactions) was introduced in Ref. [21], where, as in the HMF model, long-lived quasi-stationary states (QSSs) were found, with a duration increasing with system size. Later, inspired by the α -XY model, an interaction term decaying with distance as $r^{-\alpha}$ ($\alpha \geq 0$) was introduced in one-

dimensional chains of rotators [23]. The duration of the QSS decreases with α until its disappearance in the short-range regime, like in the α -XY model. Finally, in Ref. [24], d -dimensional lattices were studied, and q -Gaussian distributions for the time-averaged momenta and q -exponential distributions for the time-averaged energies were obtained, with values of q depending on the ratio α/d . The same type of α/d dependence was again obtained for the exponent κ governing the scaling of the Lyapunov exponent with system size. Here we further study this model, focusing now on the dependence of the QSS duration on the size N , α , and d .

II. THE MODEL

The α -Heisenberg inertial model consists of N interacting rotators, represented by three-component rotating vectors $\vec{S}_i$ with unit norm, located at fixed positions on a d -dimensional hypercubic lattice of linear size L ($N \equiv L^d$). The dimensionless ferromagnetic Hamiltonian is given by

$$\mathcal{H} = K + V_\alpha = \frac{1}{2} \sum_{i=1}^N \vec{L}_i^2 + \frac{1}{2\bar{N}} \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N \frac{1 - \vec{S}_i \cdot \vec{S}_j}{r_{ij}^\alpha}, \quad (1)$$

where the kinetic and potential energies K and V_α depend on time t .

Moreover, $\alpha \geq 0$ controls the interaction range, r_{ij} denotes the distance between rotators i and j , and the angular momenta $\vec{L}_i$ coincide with the angular velocities since we are considering unit moments of inertia. The prefactor with $\bar{N}(\alpha, d) \equiv \sum_{j \neq i} \frac{1}{r_{ij}^\alpha}$ in the potential energy is currently included in order to get a total potential energy V_α which scales linearly with N , like the total kinetic energy, so that the total energy is extensive [12]. It is straightforwardly verified that $\bar{N}(\alpha, d)$ scales, for $N \rightarrow \infty$, like $N^{1-\alpha/d}$, $\ln N$, and constant for $0 \leq \alpha/d < 1$, $\alpha/d = 1$, and $\alpha/d > 1$, respectively. It is easily seen that, for $\alpha = 0$ (infinite-range case), $\bar{N}(0, d) = N - 1 \approx N$, thus recovering the traditional mean-field-approach prefactor.

The restriction $i \neq j$ may be dismissed since $\vec{S}_i^2 = 1$, hence the total potential energy satisfies

$$V_0 = \frac{N}{2} (1 - M^2), \quad (2)$$

where the order parameter M is the norm of the total magnetization $\vec{M} = \frac{1}{N} \sum_{i=1}^N \vec{S}_i$.

Furthermore, following the usual prescription for the definition of kinetic temperature, $T(t) = \frac{2}{nN} \langle K(t) \rangle = \frac{1}{N} \langle K(t) \rangle$, where $n = 2$ represents the number of kinetic degrees of freedom per particle (three components of the spin vector minus the constant norm restriction, in variance with the classical XY model, for which we have $n = 1$), and the average is done over initial conditions. Thus, considering the energy per particle $U \equiv \frac{\langle \mathcal{H} \rangle}{N}$ in Hamiltonian (1) with $\alpha = 0$ together with Eq. (2), we obtain

$$U = T + \frac{1}{2} (1 - M^2). \quad (3)$$

This relation, together with the consistency equation for the magnetization [1,2]

$$M = \mathcal{L}(M/T), \quad (4)$$

with the Langevin function $\mathcal{L}(x) \equiv \coth x - \frac{1}{x}$, determines a relation between the thermodynamical variables of the model, which undergoes a second-order phase transition for the critical values $(T_c, U_c) = (\frac{1}{3}, \frac{5}{6})$. In the paramagnetic phase the order parameter vanishes, so introducing $M = 0$ in Eq. (3), one obtains $U = T + \frac{1}{2}$. The caloric and the M - T curves and some other details can be found in Ref. [23]. It can be shown [15] that, within BG statistical mechanics, Eqs. (3) and (4) are not only valid for $\alpha = 0$ but also throughout the $0 \leq \alpha/d \leq 1$ regime.

No analytical results are available in the short-range regime except for the limiting case $\alpha \rightarrow \infty$, which corresponds to nearest-neighbors interactions, where $\bar{N}(\infty, d) = 2d$ (number of nearest-neighbor spins on a d -dimensional hypercubic lattice) and the potential energy reduces to

$$V_\infty = \frac{1}{2d} \sum_{\langle i, j \rangle} (1 - \vec{S}_i \cdot \vec{S}_j), \quad (5)$$

where $\langle i, j \rangle$ indicates that sites labeled i and j are nearest neighbors. The $d = 1$ internal energy reads

$$U = T + \frac{1}{2} [1 - \mathcal{L}(1/2T)], \quad (6)$$

while $M = 0 \forall T \neq 0$ (no phase transition in the $d = 1$ short-range regime).

From the definition $\vec{L}_i = \vec{S}_i \times \dot{\vec{S}}_i$ one trivially obtains $\dot{\vec{S}}_i = \vec{L}_i \times \vec{S}_i$. In addition $\dot{\vec{L}}_i = \vec{S}_i \times \ddot{\vec{S}}_i = -\vec{S}_i \times \frac{\partial V_\alpha}{\partial \vec{S}_i}$, hence

$$\dot{\vec{S}}_i = \vec{L}_i \times \vec{S}_i, \quad (7)$$

$$\dot{\vec{L}}_i = \vec{S}_i \times \vec{M}_i, \quad (8)$$

where

$$\vec{M}_i \equiv -\frac{\partial V_\alpha}{\partial \vec{S}_i} = \frac{1}{\bar{N}} \sum_{j \neq i}^N \frac{\vec{S}_j}{r_{ij}^\alpha}, \quad (9)$$

reflects the interactions of spin i with the other $(N - 1)$ spins. This quantity becomes the total magnetization $\vec{M}$ when $\alpha = 0$, and the sum $\frac{1}{2d} \sum_{\langle i, j \rangle} \vec{S}_j$, extended to the nearest neighbors of spin i , when $\alpha = \infty$. Equations (7) and (8) imply not only the aforementioned conservation of the spin norms, since $\vec{S}_i^2 = 2\vec{S}_i \cdot \dot{\vec{S}}_i = 2\vec{S}_i \cdot (\vec{L}_i \times \vec{S}_i) = 0$, but also the conservation of the total angular momentum $\vec{L} = \sum_{i=1}^N \vec{L}_i$, since $\dot{\vec{L}} = \sum_{i=1}^N \dot{\vec{L}}_i = \frac{1}{N} \sum_{i=1}^N \sum_{j \neq i}^N \frac{\vec{S}_i \times \vec{S}_j}{r_{ij}^\alpha} = \vec{0}$.

III. RESULTS

We numerically integrated Eqs. (7) and (8). The N rotators are localized on sites of d -dimensional lattices ($d = 1, 2$, and 3) of linear sizes L , with periodic boundary conditions, with r_{ij} being defined as the smallest distance between sites i and j ; it follows that $N = L$ (ring), $N = L^2$ (square lattice torus), and $N = L^3$ (simple cubic lattice hyper-torus). The total number of rotators were chosen for convenience; namely, $N = 15625$, $46\,656$, $117\,649$, $262\,144$, $531\,441$, and 10^6 , which may all be written in the form $N = L^d$ for $d = 1, 2, 3$. We used the fast Fourier transform algorithm and the standard fourth-order Runge-Kutta algorithm with an integration step $h = 0.05$. The

FIG. 1. Kinetic temperature, $T(t) = \langle K(t) \rangle / N$ versus time t for $\alpha/d = 0.9$, for widely different values of N on d -dimensional lattices ($d = 1, 2$ and 3) of linear sizes L , with $N = L^d$. Notice that the duration of the QSS increases with N and d .

energy per particle was fixed at $U = 0.76$ and is conserved a long time within a relative precision of 10^{-4} .

As initial conditions, we take random sets of angular momenta, $\{\tilde{L}_i\}$, with components drawn from a symmetric uniform distribution and then redefined in order to yield zero total momentum. As for the spins $\{\tilde{S}_i\}$, two of their components are randomly chosen, while the third one is obtained by the orthogonality restriction $\tilde{S}_i \cdot \tilde{L}_i = 0$ ($\forall i$). Then, we get spins of unit length dividing by the norm. Finally, the angular momenta are rescaled so as to obtain the desired total energy per particle U . This process yields a nearly vanishing initial magnetization [i.e., $\tilde{M}(0) \simeq 0$ and $V_\alpha(0) \simeq 0.5$].

Figure 1 exhibits the time evolution of the kinetic temperature $T(t)$ for systems of rotators on d -dimensional lattices, with sizes as defined above and interactions characterized by $\alpha/d = 0.9$ (long-range regime). It is clearly observed that the duration t_{QSS} of the QSS increases with both N and d . For fixed d , the infinite time and the thermodynamic limits do not commute: (i) Taking first the $t \rightarrow \infty$ limit, one obtains $\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} = T_{\text{BG}}$, with $T_{\text{BG}} = 0.3118$, obtained from Eqs. (3) and (4) for $U = 0.76$; (ii) On the other hand, taking first the thermodynamic limit, the system would remain forever in the QSS, never attaining the final BG equilibrium temperature, since one obtains $\lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty} = T_{\text{QSS}}$, with $T_{\text{QSS}} = U - \frac{1}{2} = 0.26$, obtained as a prolongation of the linear part of the caloric curve into the nonlinear one. This non-commutativity reflects the nonergodicity of the model in the long-range regime [12].

Figure 2 exhibits the duration of the QSSs shown in Fig. 1, defined as the time interval up to the midpoint between T_{QSS} (temperature of the first plateau) and T_{BG} (temperature of the second plateau), conveniently rescaled and exhibited versus N . Straight lines fit well to the data and strongly suggest that

$$t_{\text{QSS}} = [\lambda(\alpha/d)]^{d-1} \mu(\alpha/d) N^{A(\alpha/d)} \quad (d = 1, 2, 3). \quad (10)$$

The prefactor $[\lambda(\alpha/d)]^{d-1}$ becomes necessary as α/d approaches the short-range regime (in fact, $\lambda \simeq 1.16$ for $\alpha/d = 0.8, 0.9$ and $\lambda = 1$ otherwise). Consistently, by representing

FIG. 2. The durations of the QSSs of Fig. 1, as well as of others corresponding to different values of α/d , can be rescaled conveniently with $t_{\text{QSS}} = [\lambda(\alpha/d)]^{d-1} \mu(\alpha/d) N^{A(\alpha/d)}$. The straight lines fit well to the data. To collapse all the $d = 1, 2, 3$ data we have used $\lambda = 1$, excepting for $\alpha/d = 0.8, 0.9$; indeed, their proximity to the short-range threshold, where no such collapse can exist, has demanded $\lambda = 1.16$. It is expected that, in the thermodynamic limit, λ approaches unity for all $0 \leq \alpha/d \leq 1$. (inset) We verify that the exponent A appears to depend linearly on $(\alpha/d)^2$.

the kinetic temperatures $T(t)$ of Fig. 1 versus t/t_{QSS} , one notices that the QSS temperatures nearly collapse in the mid-height region, $\forall (d, N)$ (see Fig. 3).

We investigate now how t_{QSS} depends on α/d , for fixed N . Figure 4 shows $T(t)$ for fixed N ($N = 15625$, following $N = L^d$, with $d = 1, 2$, and 3) and increasing values of α/d . Notice that t_{QSS} decreases for increasing α/d ($0 \leq \alpha/d < 1.0$), with the QSS typically disappearing whenever approaching the short-range regime. In this regime we do not expect data collapse among different values of d , since these are known to represent distinct physical systems, characterized by peculiar properties. For example, at equilibrium, a ferromagnetic phase

FIG. 3. Kinetic temperature $T(t)$ of Fig. 1 now represented versus t/t_{QSS} , through Eq. (10). The double arrow at mid-height (0.2859) characterizes the numerical abscissa spread of the collapse (from 0.85 to 1.15).

FIG. 4. The kinetic temperature, $T(t) = \langle K(t) \rangle / N$, is represented versus time t (on a logarithmic scale) for a fixed number of rotators ($N = 15\,625$, following $N = L^d$, with $d = 1, 2$, and 3) and increasing values of α/d ($\alpha/d = 0, 0.1, 0.2, \dots, 1.3, 1.5$, and 2.0). Notice that t_{QSS} decreases for values of α/d increasing from zero up to unity, above which the QSS disappears.

appears at low temperatures for $d = 3$, but not for $d = 1$ and 2 [1,2]. Indeed, as shown in Fig. 4, while the long-time-limit temperature, T_{BG} , is the same for values of α/d in the long-range regime, it depends on d in the short-range regime.

Figure 5 exhibits the duration of the QSSs shown in Fig. 4 versus $(\alpha/d)^2$ in a log-linear plot. Considering several values of α/d ($0 \leq \alpha/d \leq 0.8$), the fits yield a Gaussian dependence, i.e., $t_{\text{QSS}} \propto \exp[-B(N)(\alpha/d)^2]$. Figure 6 exhibits $T(t)$ shown in Fig. 4 versus t/t_{QSS} , with t_{QSS} following a Gaussian; namely, $t_{\text{QSS}} = [\lambda(\alpha/d)]^{d-1} \nu(N) \exp[-B(N)(\alpha/d)^2]$, with $B(N) = 1.33 N^{0.19}$, as indicated in Fig. 5.

FIG. 5. The durations, for $d = 1, 2, 3$, of the QSSs shown in Fig. 4 (open circles) are represented versus $(\alpha/d)^2$ in a log-linear plot. The full straight lines represent best fits for the data. (inset) N dependence of B .

Figure 7 combines Figs. 2 and 5 into a single plot, showing an approximate collapse of 24 different $T(t)$ curves: two values of N ($N = 15\,625$ and $46\,656$, following $N = L^d$, with $d = 1, 2$, and 3) and four values of α/d ($\alpha/d = 0.5, 0.6, 0.7$, and 0.8). The results in Fig. 7 suggest the following scaling:

$$\frac{t_{\text{QSS}}(N, \alpha, d)}{[\lambda(\alpha/d)]^{d-1}} = \nu(N) \mu(\alpha/d) N^{A(\alpha/d)} e^{-B(N)(\alpha/d)^2}, \quad (11)$$

with $A(\alpha/d) \simeq 1.8 - 1.5 (\alpha/d)^2$, $B(N) \simeq 1.33 N^{0.19}$, $\mu(\alpha/d)$ and $\nu(N)$ are defined in Figs. 2 and 5, respectively, $\lambda(\alpha/d)$

FIG. 6. The numerical data for the kinetic temperature $T(t)$ of Fig. 4 ($0 \leq \alpha/d \leq 0.8$) are now represented versus t/t_{QSS} , by considering the Gaussian behavior $t_{\text{QSS}} \propto \exp[-B(N)(\alpha/d)^2]$. The double arrow at mid-height (0.2859) characterizes the numerical abscissa spread of the collapse (from 0.8 to 1.2).

FIG. 7. Kinetic temperature $T(t)$ versus the scaled variable t/t_{QSS} for typical values of N ($N = 15\,625$, and $46\,656$), α/d ($\alpha/d = 0.5, 0.6, 0.7, 0.8$), and $d = 1, 2$, and 3 , through Eq. (11). The double arrow at mid-height (0.2859) characterizes the numerical abscissa spread of the collapse (from 0.8 to 1.2).

remains equal to unity for $0 \leq \alpha/d < 0.8$ and close to 1.16 for $\alpha/d = 0.8, 0.9$. Concerning A , notice that, (i) for long-range XY ferromagnets, the value $A \simeq 0.6$ has been obtained [19] for the QSS plateau; and (ii) for long-range Fermi-Pasta-Ulam models, the value A corresponding to the BG- q crossover time t_c is given by $A \simeq 1/1.365 \simeq 0.73$ [25].

IV. CONCLUSIONS

We studied, through first-principle simulations, the d -dimensional classical inertial Heisenberg ferromagnet with a two-body interaction decaying as $1/r_{ij}^\alpha$ ($\alpha \geq 0$), focusing on the duration t_{QSS} of the QSS appearing before a crossover to a second plateau, corresponding to the BG temperature T_{BG} , although *not* to the BG equilibrium state. We obtain that t_{QSS} increases with the number N of rotators as N^A , which, combined with a Gaussian-like decay with α/d , yields the scaling indicated in Eq. (11). To our knowledge, this represents the first thorough investigation of how the duration of t_{QSS} depends on (N, α, d) ; minor variations are expected to occur by changing the specific class of initial conditions at a given internal energy U , as well as for different values of U itself. One always comes across with the basic question on which specific quasi-stationary state we are focusing on and how time scales. The present results should guide future investigations on other long-range Hamiltonian systems, such as gravitation, the α -XY, Coulombian, α -Lennard-Jones models, among others. We expect this to be so either through numerical simulations, or analytical calculations, and even possibly in experiments (see, for instance, Ref. [26]).

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