Time average and canonical average of macroscopic variable in classical Hamiltonian system with long-range interaction

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abstract

We study finite size effects in a family of classical Hamiltonian systems in which a parameter controls interaction-range. In the long-range regime where the infinite-size free energy is universal, we show that the finite size effects are not universal but depend on the interaction-range. The finite size effects are observed through discrepancies between time-averages of macroscopic variables in Hamiltonian dynamics and canonical averages of ones with infinite degrees of freedom. For a high energy regime, the relation to a pair of the discrepancies is theoretically predicted and numerically confirmed.

要旨

相互作用距離が1パラメータでコントロールされる大自由度古典ハミルトン力学系族を調べた．この力学系族の長距離力領域においては，自由エネルギーは熱力学極限で相互作用距離に依らないが，リアプノフ数の自由度依存性は相互作用距離に依存することが知られている．今回我々はマクロ変数の自由度依存性に注目し，ハミルトン力学による時間平均値と，熱力学極限でのカノニカル平均値との相違を観察することにより有限サイズ効果の相互作用距離依存性を調べた．この有限サイズ効果を高エネルギー領域で理論的に予言し，数値的に確認することができた．

1 Introduction

In many body systems, the range of interactions governs physical features. Long-range interactions induce a phase transition, and typical ones are the mean-field interactions. For instance, the Hamiltonian mean-field (HMF) model which consists of planar rotators shows a second-order phase transition between a low energy ordered phase and a high energy disordered phase [1]. On the other hand, short-range interactions are hard to occur the phase transition, particularly in low-dimensional systems.

To investigate how the range of interactions affects the existence of a phase transition, the HMF model is extended to a model having algebraically decaying interactions, called the α-XY model, described by the following Hamiltonian [2]:

$$H = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2\tilde{N}}\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{1-\cos(q_i-q_j)}{r_{ij}^{\alpha}}. \tag{1}$$

Each rotator is placed on a site of the periodic d-dimensional simple lattice, that is $N = L^d$ for the lattice of size L, and r_{ij} is the shortest distance between the sites i and j. The α-XY model includes the HMF model as $\alpha = 0$, and the nearest neighbor interaction realizes in $\alpha \to \infty$. The factor $\tilde{N}$ is introduced for recovering the extensivity of the system, but the factor does not make the system additive for $0 \leq \alpha/d < 1$. In this article, $\tilde{N}$ is defined as $\sum_{i=1}^{N} 1/r_{ij}^{\alpha}$ [3]. In the long-range regime $0 \leq \alpha/d < 1$, Campa *et al.* show that the α-XY model including the external magnetic field essentially has the same canonical partition function with the HMF model in $N \to \infty$[3], and the critical value of the energy for a second-order phase transition is common as $U = E/N = 0.75$, E being the value of the Hamiltonian. Recent studies of the α-XY model are briefly summarized in Ref.[4].

In this article, in the long-range regime, we investigate how macroscopic variables for the α-XY system with finite N approaches the thermodynamic limit ($N \to \infty$). They could go towards canonical averages as N increases [5, 6, 7], but it is not obvious whether the convergence speed depends on α/d or not. Some non-universalities appear as dynamical aspects in $0 \leq \alpha/d < 1$ [4], and hence we compare canonical averages of the macroscopic variables in $N \to \infty$ and time-averaged variables with N. The latters are obtained by integrating the canonical equation of motion yielded from the Hamiltonian (1). We set $d = 1$ for the convenience of numerical computations, and show that, for the supercritical energy regime, the time-averages of macroscopic variables with finite N algebraically approach the canonical averages taken in $N \to \infty$ as N increases, and the exponents depend on α.

2 Theoretical Prediction

As macroscopic variables we observe, we adopt modulus of the magnetization and the temperature. The magnetization vector $\vec{M} := (M_x, M_y)$ and its modulus M are defined as $\vec{M} := \sum_{i=1}^{N}(\cos q_i, \sin q_i)/N$ and $M := \sqrt{M_x^2 + M_y^2}$, respectively. The temperature in the sence of dynamics is defined as $T_N^d := \sum_{j=1}^{N} p_j^2/N$. Note that we numerically compute averages through Hamiltonian dynamics instead of canonical ensemble, then a fixed variable is neither T nor T_N^d, but the internal energy $U = E/N$.

In this section, we estimate the following two discrepancies

$$\delta_M(N) := \langle M \rangle_N - \langle M \rangle_\infty, \quad \delta_T(N) := T_N - T, \tag{2}$$

where $\langle X \rangle_N$ and $\langle X \rangle_\infty$ denote the canonical average of X with finite N degrees of freedom and one in $N \to \infty$ respectively. $\langle U \rangle_N$ and $\langle M \rangle_N$ are calculated in Ref [8] with the aid of the saddle-point approximation[3]. T_N is the temperature for the system with N degrees of freedom and is defined as

$$U = \langle U \rangle_N (T_N). \tag{3}$$

The relation (3) bridges between Hamiltonian dynamics and canonical statistics. We require that the relation (3) holds in any degrees of freedom and hence $\langle U \rangle_N (T_N) = \langle U \rangle_\infty (T)$. The average $\langle U \rangle_\infty (T)$ is related to T and $\langle M \rangle_\infty^2$ as

$$2\langle U \rangle_\infty (T) = T + 1 - [\langle M \rangle_\infty (T)]^2. \tag{4}$$

The relation (4) is straightforwardly obtained for the HMF model, and holds in the long-range regime $0 \leq \alpha < 1$ due to the universality of the canonical partition function [3].

Although we do not show the derivation, we can show the following relation for $T \geq T_c$ [8]

$$\delta_T(N) = [\delta_M(N)]^2 + bN^{-(1-\alpha)}. \tag{5}$$

The constant b represents the diagonal elements of the matrix $(1/r_{ij}^{\alpha})$, and can be chosen arbitrarily. We select $b = 2.0$ to obtain a fully positive spectrum which enables us to apply the Hubburd-Stratonovitch transformation [3].

3 Numerical Results

Let us check the validity of our theoretical predictions of δ_T and δ_M numerically. The time-averaged temperature $\langle T_N^d \rangle_t$ and the order parameter $\langle M \rangle_t$ are defined as follows:

$$\left\langle T_N^d \right\rangle_t (t_0) := \frac{1}{t_0} \int_0^{t_0} T_N^d(t)\, dt, \quad \langle M \rangle_t (t_0) := \frac{1}{t_0} \int_0^{t_0} M(t)\, dt. \tag{6}$$

Numerical integrations of the canonical equation of motion are performed by using a fourth-order symplectic integrator. Thanks to the Fast Fourier Transformation technique, the calculation times are of order $N \ln N$. The time slice of the integrator is set at 0.2 and it suppresses the relative energy error $\Delta E/E \sim 10^{-5}$. Our initial condition is, for all values of α, the canonical equilibrium distribution of the HMF model, that is p and q are randomly taken from the distributions being proportional to $\exp(-\beta p^2/2)$ and $\exp(\beta \langle M \rangle_\infty \cos q)$ [7] respectively. The total momentum is an integral of motion, and we initially set it to zero. The computing time, t_0 in Eq.(6), are set to more than 10^6 to realize equilibrium states in the sense of dynamics, where we define such equilibrium as when the time-averaged macroscopic variables are almost stational.

For the supercritical energy regime, we investigate the finite size effects for two values of energy. One is the high enough energy $U = 5.0$, and the other one is supercritical but the middle energy $U = 0.8$. The discrepancies $\delta_M(N)$ and $\delta_T(N)$ are shown in Fig.1 as functions of N. It is shown that the discrepancies algebraically decrease as N increases, that is

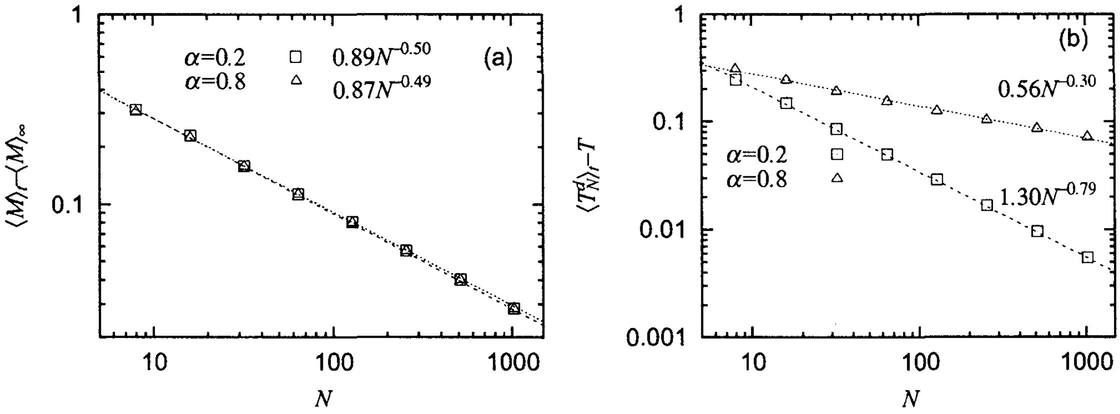

Fig. 1: Dependence on N of the two discrepancies (a) $\langle M \rangle_t - \langle M \rangle_\infty$ and (b) $\langle T_N^d \rangle_t - T$ at $U = 5.0$. Asymptotic power-law decays are observed.

$$\delta_M(N) \propto N^{-\mu_M(\alpha,U)}, \quad \delta_T(N) \propto N^{-\mu_T(\alpha,U)}. \tag{7}$$

According to the theoretical prediction (5), the exponent μ_M should be related to the other μ_T as

$$\mu_T = \min(2\mu_M, 1-\alpha). \tag{8}$$

Let us check the relation (8) by observing the exponents μ_M and μ_T as functions of α.

For the high enough energy $U = 5.0$ (see Fig.2(a)), the theoretical curve is in good agreement with numerical results in the interval $0 \leq \alpha \lesssim 0.6$. In addition, the theoretical prediction is qualitatively good for $U = 0.8$ (see Fig.2(b)). For further discussions, we refer the reader to Ref.[8].

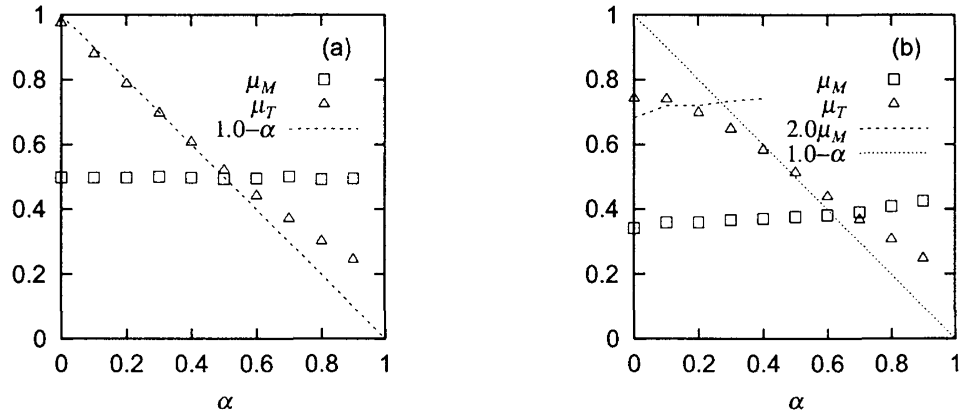

Fig. 2: Exponents μ_M and μ_T as functions of α. (a) $U = 5.0$. (b) $U = 0.8$. Dashed curves represent theoretical predictions.

4 Conclusions

In this article the α-XY model (1) with $d = 1$ has been studied for the long-range regime $0 \leq \alpha < 1$, so that we clarify the role of interaction length in Hamiltonian systems with many degrees of freedom[8]. We have studied dependences on degrees of freedom for time-averaged macroscopic variables calculated through Hamiltonian dynamics with finite degrees of freedom, contrasted with the canonical averages of ones in the thermodynamic limit. A non-universal behavior in $0 \leq \alpha < 1$ is observed in the asymptotic behavior of the discrepancies for the supercritical regime. For the supercritical regime, the discrepancy between the two averages decays as a power-type function, and the exponents depending on α are explained by applying the canonical ensemble with finite degrees of freedom with the aid of the saddle-point approximation. This non-universal behavior sheds light on the study of Hamiltonian systems with long-range interactions.

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