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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.

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 $\alpha$-XY model, described by the following Hamiltonian [2]:

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

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 $\alpha$-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 $\sum_{i=1}^{\tilde{N}} 1/r_{ij}^2$ [3]. In the long-range regime $0 \leq \alpha/d < 1$, Campa et al. show that the $\alpha$-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 $\alpha$-XY model are briefly summarized in Ref.[4].

In this article, in the long-range regime, we investigate how macroscopic variables for the $\alpha$-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 $\alpha/d$ 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 latter 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 $\alpha$.

2 Theoretical Prediction

As macroscopic variables we observe, we adopt modulus of the magnetization and the temperature. The magnetization vector $\tilde{M} := (M_x, M_y)$ and its modulus $M$ are defined as $\tilde{M} := \sum_{i=1}^{\tilde{N}} (\cos q_i, \sin q_i)/N$ and $M := \sqrt{M_x^2 + M_y^2}$, respectively. The temperature in the sense 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

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

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

$$
U = \langle U \rangle_N (T_N).
$$

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

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

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]

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

The constant $b$ represents the diagonal elements of the matrix $(1/r_{ij}^2)$, and can be chosen arbitrarily. We select $b = 2.0$ to obtain a fully positive spectrum which enables us to apply the Hubbard-Stratonovitch transformation [3].

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3 Numerical Results

Let us check the validity of our theoretical predictions of $\delta_T$ and $\delta_M$ numerically. The time-averaged temperature $\langle T_N^2 \rangle_t$ and the order parameter $\langle M \rangle_t$ are defined as follows:

\[
\langle T_N^2 \rangle_t (t_0) := \frac{1}{t_0} \int_0^{t_0} T_N^2(t) \, dt, \quad \langle M \rangle_t (t_0) := \frac{1}{t_0} \int_0^{t_0} M(t) \, dt.
\]

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 $\alpha$, 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 $\exp(\beta M \cos q)$ [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 stationary.

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

\[
\delta_M(N) \propto N^{-\mu_M(\alpha, U)}, \quad \delta_T(N) \propto N^{-\mu_T(\alpha, U)}.
\]

Fig. 1: Dependence on $N$ of the two discrepancies (a) $\langle M \rangle_t - \langle M \rangle_{\infty}$ and (b) $\langle T_N^2 \rangle_t - T$ at $U = 5.0$. Asymptotic power-law decays are observed.

According to the theoretical prediction (5), the exponent $\mu_M$ should be related to the other $\mu_T$ as

\[
\mu_T = \min(2\mu_M, 1 - \alpha).
\]

Let us check the relation (8) by observing the exponents $\mu_M$ and $\mu_T$ as functions of $\alpha$.

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 $0 \leq \alpha \leq 0.6$. 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].
4 Conclusions

In this article the $\alpha$-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 $\alpha$ 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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