Methods of exploring energy diffusion in lattices with finite temperature

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Abstract

We discuss two methods for exploring energy diffusion in lattices with finite temperature in this paper. The first one is the energy-kick (EK) method. To apply this method, one adds an external energy kick to a particle in the lattice, and tracks its evolution by evolving the kicked system. The second one is the fluctuation-correlation (FC) method. This method is presented recently by one of the present authors [Zhao, Phys. Rev. Lett. **86**, 11003 (2006)]. In present paper, the formula for calculating the probability density function (PDF) using the canonical ensemble is slightly revised and extended to the microcanonical ensemble. To apply the FC method, one tracks the motion of the energy initially localized at a small region by a properly constructed correlation function of energy fluctuations. Both methods can obtain a PDF of energy diffusion. However, we show that the FC method has advantages over the EK method theoretically and technically. Theoretically, the PDF obtained by the FC method reveals the diffusion processes of the inner energy while the PDF obtained by the EK method represents that of the kick energy. The diffusion processes of the inner energy and the external energy added to the system, i.e., the kick energy, may be different quantitatively and even qualitatively depending on models. To show these facts, we study not only the equilibrium systems but also the stationary nonequilibrium systems. Examples showing that the inner energy and the kick energy may have different diffusion behavior are reported in both cases. Technically, since applying the energy fluctuations of particles in the system, a set of independent realizations to the ensemble average can be achieved by one round of evolution of the system when applying the FC method. This advantage enables us to study the long-time diffusion processes in large-scale systems and thus avoids the finite-time effect.

PACS numbers: 05.60.-k, 44.10.+i

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I. INTRODUCTION

Diffusion is one of the most important types of motion in nature. According to the time-dependent behavior, $\langle r^2(t)\rangle \sim t^\alpha$, of the mean square displacement of a conserved quantity, it is classified as subdiffusion ($\alpha < 1$), normal diffusion ($\alpha = 1$) and superdiffusion ($\alpha > 1$) [1, 2]. Among various quantities, the diffusion of particle and the diffusion of energy have particular importance both for theoretical studies and applications. The diffusion of particles represents the transport behavior of mass, while the diffusion of energy determines the transport of heat. In studying the particle diffusion, one can directly calculate the PDF by tracking the motion of particles. This method has been widely used [3, 4]. However, this method is not available for energy diffusion, because a particle can be tagged and tracked while energy may not be. Therefore, developing methods to track energy diffusion is highly desirable. This is particularly important for a lattice system since particles in the system oscillate around their stationary positions and thus is not a diffusion process.

The key task of characterizing a diffusion process is to obtain the probability density function (PDF) of the related quantity, by which one can calculate the time-dependent behavior of the mean square displacement and thereby obtain the diffusion exponent α. This exponent is not only served to classify diffusion types but also to check certain theoretical predictions. In the past decade, the heat conduction problem in low-dimensional systems has attracted intensive attentions [5, 6]. It is found that some one-dimensional lattices may show anomalous heat conduction behavior [7–11]. The thermoconductivity κ in such a system depends on the lattice size N as $\kappa \sim N^\beta$. While some other one-dimensional lattices show normal heat conduction behavior [12–16]. In recent years, several groups investigated the relation between the exponents α and β [17–22], and derived equations to describe their relationship. Establishing deterministic relation between the two exponents has theoretical importance. Actually, this attempt is stimulated by the celebrated equation obtained by Einstein [23] who derived the deterministic relation between the diffusion coefficient and the coefficient of viscosity, correlating the two different irreversible processes. However, up to now, different relationship equations of α and β coexist [17, 18]. Which one describes the correct relationship, and even whether the correct one has been found, are still open problems. To answer these questions, the exponents α and β should be calculated with sufficient precision after getting rid of the size effect or finite-time effect. As shown in Ref. [24–26], the size effect of β disappears in the FPU-β lattices until $N \sim 10^3 - 10^4$. This fact reminds one that

the diffusion time should be long enough to avoid the finite-time effect on the exponent α.

Two different methods have been presented for calculating the PDF of energy diffusion. The first one is a straightforward method [19, 20, 22, 27–29]. The idea is to add a high-energy kick to a particle at a fixed position and then, after a period and at other positions, calculate the ensemble average of the difference between the current energy density and the average energy density before the kick. It is clear that the ensemble average represents the amount of kick energy transported to these positions. We call it the energy-kick (EK) method. The EK method indeed manifests the diffusion of the kick energy. The second way is presented by one of the present authors, H. Zhao, recently [21]. The basic idea is to track the motion of a part of energy by investigating a properly constructed correlation function of energy fluctuations. We call it the fluctuation-correlation (FC) method. Unlike the EK method, it studies the energy fluctuations of particles in the system. Some groups have realized that this method is more reasonable than the EK method [22, 30].

The purpose of this paper is, on one hand, to make a detailed comparison between the EK method and the FC method. We argue that the two methods indeed explore different diffusion processes. That is to say, the EK method describes the relaxation process of the kick energy or the diffusion behavior of the energy externally added to the system, while the FC method represents the diffusion behavior of the inner energy or the intrinsic diffusion behavior of the energy in the system. In certain systems, the memory of the history will be lost quickly with time evolution. In this case, the diffusion of the kick energy and the inner energy has no qualitative difference, though the PDFs obtained by the two method still have quantitative difference since the diffusion of the kick energy depends on the amplitude of kicks. In other systems, the memory of the history is not totally lost. In this case, the kick energy and the inner energy may include different information. For most lattices in equilibrium with uniform temperature, the kick energy and the inner energy diffuse in a symmetric way, and the PDFs obtained by both methods are qualitatively similar. These lattices usually have symmetric interaction potentials. While for lattices with asymmetric interaction potentials, the inner energy and the kick energy may diffuse in different ways. The PDFs obtained by the FC method are symmetric and those obtained by the EK method may be asymmetric. In nonequilibrium lattices with stationary temperature gradients, even for those lattices with symmetric interaction potentials, the PDFs obtained by the two methods may be different qualitatively. Therefore, we consider not only the energy diffusion in equilibrium systems but also in nonequilibrium systems.

On the other hand, we further explain the rationale of the FC method and describe the technical

details for applying this method. We present formulae for the canonical ensemble and the micro-canonical ensemble respectively to calculate PDFs of energy diffusion. A formula suitable for the canonical ensemble has been presented in [21]. The one presented here is slightly different from the old one. We explain that the new formula is more reasonable. Also we emphasize that the FC method has great technique advantage over the EK method. The technical disadvantage of the EK method has been pointed out in [19]. The FC method can shorten the computation time by several orders comparing with that with the EK method.

The paper is managed as follows. In next section we introduce the two methods for studying energy diffusion in equilibrium one-dimensional lattices. The rationale of the FC method is explained and the strategy for applying this method is described. An example showing the qualitative difference between the inner energy and the kick energy is reported. Section III is contributed to investigating the energy diffusion in stationary nonequilibrium lattices, i.e., in one-dimensional lattices with stationary heat flux and stationary temperature gradients. This section further reveals the diffusion behavior difference between the inner energy and the kick energy. The last section is the conclusion and the discussion of the paper.

II. ENERGY DIFFUSION IN EQUILIBRIUM LATTICES

A one-dimensional lattice is usually described by the Hamiltonian

$$H = \sum_{i=1}^{N} H_i,\ H_i = \frac{p_i^2}{2m} + U(x_i) + V(x_i - x_{i-1}),$$

where $U(x_i)$ denotes the on-site potential and $V(x_{i+1} - x_i)$ the interaction potential. In the present paper we study two types of the lattice models, without or with on-site potentials. The illustrating examples include the FPU-β model with

$$H_i = \frac{p_i^2}{2m} + \frac{1}{2}(x_i - x_{i-1})^2 + \frac{1}{4}(x_i - x_{i-1})^4$$

and the lattice ϕ^4 model with

$$H_i = \frac{p_i^2}{2m} + \frac{1}{2}(x_i - x_{i-1})^2 + \frac{1}{4}x_i^4.$$

Without loss of generality, we set mass $m = 1$, and the Boltzmann constant $k_B = 1$ in following discussions. Fixed boundary condition is applied for both models. We also employ occasionally

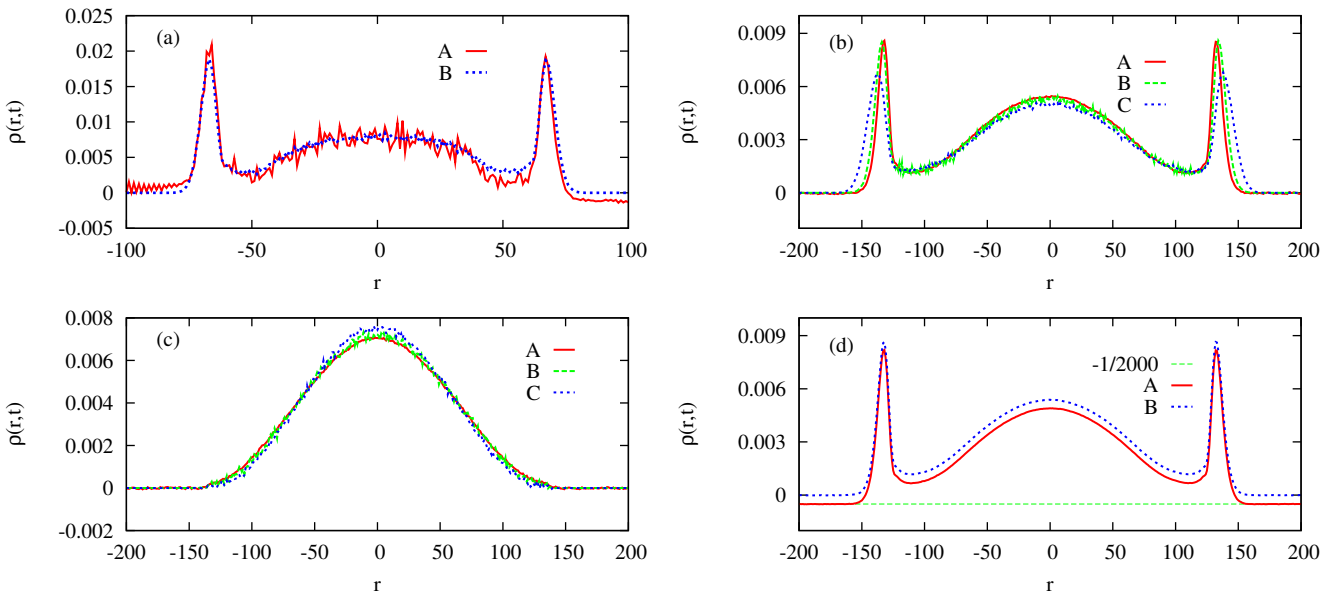

FIG. 1: (color online). The PDFs of energy diffusion at $T = 0.5$. (a) The PDFs at $t = 50$ obtained by the EK method (A) and the improved EK method (B) for the FPU-β model. (b) The PDFs at $t = 100$ obtained by the FC method(A), and the EK method with $\Delta\widetilde{H}_i(0) = 5E$ (B) and $\Delta\widetilde{H}_i(0) = 10E$ (C) for the FPU-β model. (c) The PDFs at $t = 200$ for the lattice ϕ^4 model. A, B and C are same as in (b). (d) The PDFs at $t = 100$ for the FPU-β model obtained by the FC method using microcanonical ensembles with eq.3(A) and with eq.4 (B). The line C gives $\rho(r,t) = -1/N$ for reference.

the harmonic model with $H_i = \frac{p_i^2}{2m} + \frac{1}{2}(x_i - x_{i-1})^2$, the Toda model with $H_i = \frac{p_i^2}{2m} + e^{-(x_i - x_{i-1})} + (x_i - x_{i-1}) - 1$ and the quartic-FPU model with $H_i = \frac{p_i^2}{2m} + \frac{1}{4}(x_i - x_{i-1})^4$ for special purposes.

When adding heat baths to the two ends of a lattice one obtains a canonical system. A canonical system is an open system and thus the total energy of the system is not conservative. When heat the lattice to a finite temperature and then take away the heat bath, one obtains a microcanonical system. A microcanonical system is an isolated system with total energy conserved. In both cases, after the stationary state is achieved, every particle has identical temperature, $T = \langle p_i^2 \rangle$, and identical average energy, $E = \langle H_i \rangle$.

The problem to be investigated is: how does the energy H_i or the energy difference $\Delta H_i = H_i - E$ initially located at the ith particle spread out over the lattice as a function of time? To find the solution to this problem, the EK method adds a kick $\Delta\widetilde{H}_i(0) = \widetilde{H}_i(0) - H_i(0)$ to the ith particle at $t = 0$, and calculate the part $\Delta\widetilde{H}_j(t)$ transported to the jth particle at time t, where $H_i(0)$ is the energy before the kick while $\widetilde{H}_i(0)$ represents the energy after the kick. It is clear that

without the external kick the ensemble average $\left\langle \widetilde{H}_j(t) \right\rangle$ should be equal to the average energy E. Therefore, the ensemble average $\left\langle \Delta\widetilde{H}_j(t) \right\rangle = \left\langle \widetilde{H}_j(t) \right\rangle - E$ can be explained as the average part of the kick energy transported to the jth particle at time t. One can thereby define

$$\rho(r,t) = \frac{\left\langle \Delta\widetilde{H}_j(t) \right\rangle}{\left\langle \Delta\widetilde{H}_i(0) \right\rangle} \tag{1}$$

as the PDF to describe the probability of the kick energy transported to the position r at time t, where $r = j - i$.

As an example, in Fig. 1(a) we show the PDF obtained by the EK method for the FPU-β model with temperature $T = 0.5$ and at $t = 50$. The ensemble average is over 4.2×10^5 different realizations. For each realization the lattice is developed to $t = 50$, starting by adding an external kick to the middle particle. For the sake of simplicity we fix the amplitude of kicks at $\Delta\widetilde{H}_i(0) = 5E$. The figure indicates that the profile of the PDF is already distinguishable, but the fluctuations are still large.

A different strategy can be applied to improve the convergence of the PDF for the EK method [22]. The idea is to copy the system before the kick as a reference system. Then add the kick to the middle particle of the original system and evolve the pair of the systems simultaneously to compute the energy difference between the two systems by $\Delta\widetilde{H}_j(t) = \widetilde{H}_j(t) - H_j(t)$, where the first term in the r.h.s is the energy of the jth particle of the kicked system while the second is that of the reference system. It is clear that the difference represents exactly the kick energy transported to the jth particle. By averaging the same amount of realizations as in above we obtained the PDF and show it also in Fig. 1(a). One can find that the fluctuations are dramatically smoothed. The PDFs obtained by the EK method hereafter are calculated using this strategy.

The EK method is presented in the spirit of the linear response theory[31], which demands the kick energy small enough to keep a linear response. However, practically, it can not be too small otherwise the fluctuations of the ensemble average will be too large. In this situation, the PDF will depend on the amplitude of the kick energy. In Fig. 1(b) we show the PDFs calculated with kicks of amplitude $\Delta\widetilde{H}_i(0) = 5E$ and of amplitude $\Delta\widetilde{H}_i(0) = 10E$. It is obvious that the kick energy with $\Delta\widetilde{H}_i(0) = 10E$ diffuses faster than that with $\Delta\widetilde{H}_i(0) = 5E$. The same effect remains in the lattice ϕ^4 model, as Fig. 1(c) shows. Nevertheless, in this model the high-energy kick diffuses slower than that of the low-energy kick, which confirms the observation that the higher of the energy, the stronger of the localization effect in this model [32]. Therefore, the EK method studies

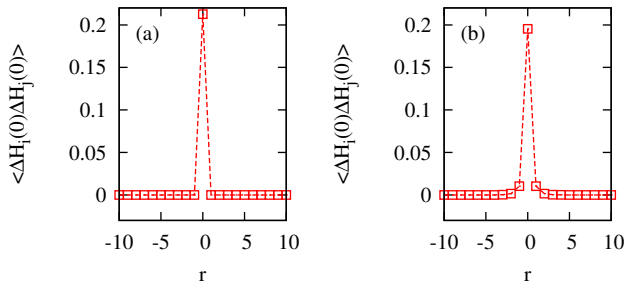

FIG. 2: (color online). The initial (spatial) correlation $\langle \Delta H_i(0) \Delta H_j(0) \rangle$ of the FPU-β model (a) and the lattice ϕ^4 model (b).

indeed the diffusion process of the kick energy; it is not directly explore the intrinsic diffusion behavior in the system.

The desirable way is to study directly the inner energy, i.e., the energy initially localized at a particle or in a small region in the lattice. The difficult is that one can not directly track this part of energy because it can not be marked, as does in the case of particle diffusion. Let $\Delta H_i(0)$ represents the energy fluctuation initially located at the ith particle. Then if a portion of $\Delta H_i(0)$ is transported to the jth particle at time t, the energy fluctuation $\Delta H_j(t)$ should have correlation with $\Delta H_i(0)$ physically. The idea of the FC method is to track the motion of the inner energy by calculating the correlation of the energy fluctuations. The first step of applying the FC method is to determine the part of energy, denoted by $\Delta H(0)$, to be studied. We show how to do this by examples. In Fig. 2(a) and 2(b), we plot $\langle \Delta H_i(0) \Delta H_j(0) \rangle$ of the FPU-β model and the lattice ϕ^4 model respectively, where $r = j - i$. Canonical systems with $N = 501$ are employed for both models. It can be seen that $\langle \Delta H_i(0) \Delta H_j(0) \rangle = 0$ (within numerical errors) for $j \neq i$ and $\langle \Delta H_i(0) \Delta H_j(0) \rangle \neq 0$ for $j = i$ for the FPU-β model, which indicate that $\Delta H_i(0)$ has no initial correlation with the energy fluctuations of other particles. In this case, we employ $\Delta H(0) = \Delta H_i(0)$ as the energy to be studied. While in the case of the lattice ϕ^4 model, it has $\langle \Delta H_i(0) \Delta H_j(0) \rangle > 0$ for several nearby particles, which implies that $\Delta H_i(0)$ is intrinsically correlated with a part of energy besides $\Delta H_i(0)$ itself. Because this part of energy can not be separated from $\Delta H_i(0)$, we have to consider it as a whole as the objective $\Delta H(0)$ to be studied. We call $\Delta H(0)$ as the adherence energy of $\Delta H_i(0)$.

It is easy to understand why in certain systems $\Delta H_i(0)$ adheres a small part of energy while in other systems it does not. In a lattice with finite temperature, at the same moment the fluctuations of the kinetic energy of particles are independent because the velocity of a particle at a

moment puts no restriction on that of other particles. For a class of lattices with only interaction potentials, such as the FPU-β model, the potential is determined by the relative displacements. A configuration of $x_i - x_{i-1}$ which determines the potential part of H_i is completely independent of the configuration of $x_{i+1} - x_i$ which determines the potential part of H_{i+1}. As a result, H_i and H_{i+1} are independent with each other and thus $\langle \Delta H_i(0) \Delta H_j(0) \rangle = 0$ for $j \neq i$. For another class of lattices with on-site potentials, such as the lattice ϕ^4 model, the situation is different. When the ith particle moves to the left/right to its equilibrium position, the neighbor particles will tends to follow it because of the interaction potential between them. This effect results in a positive correlation, i.e., the bigger the on-site potential $x_i^4/4$, the bigger the $x_{i\pm1}^4/4$, and *vice versa*.

We then define

$$\rho(r,t) = \frac{\left\langle \Delta H_i(0) \Delta H'_j(t) \right\rangle}{\langle \Delta H_i(0) \Delta H(0) \rangle} \tag{2}$$

as the PDF to describe the motion of $\Delta H(0)$. The reason is as follows. First, $\Delta H(0)$ never disappears before it spreads out of the lattice because of the energy conservation, i.e., it is a conserved quantity. Thus, one has $\sum_j \Delta H_i(0) \Delta H'_j(t) = \Delta H_i(0) \Delta H(0)$, which gives $\int \rho(r,t) dx = 1$. Second, $\Delta H_i(0)$ and $\Delta H(0)$ are positively correlated, and $\Delta H'_j(t)$ and $\Delta H(0)$ should also be positively correlated since the former is a part of the latter, one obtains $\rho(r,t) \geqslant 0$. Non-negativity and normalization conditions are basic requirements to be a PDF. Finally, it is clear that $\rho(r,t)$ is proportional to $\Delta H'_j(t)/\Delta H(0)$. Therefore, $\rho(r,t)$ can be considered as the probability of finding $\Delta H(0)$ at the position r at time t, or equally, it represents the rate of $\Delta H(0)$ to be transported to r at time t.

The problem is how to calculate $\left\langle \Delta H_i(0) \Delta H'_j(t) \right\rangle$. At time t we divide the energy fluctuation at the jth particle into two parts, i.e., $\Delta H_j(t) = \Delta H'_j(t) + \Delta H''_j(t)$, where $\Delta H'_j(t)$ represents the part of $\Delta H(0)$ being transported to the jth particle, and $\Delta H''_j(t)$ comes from other sources. For a canonical system, $\Delta H''_j(t)$ has no correlation with $\Delta H_i(0)$ since it comes from {other parts of the system or} the heat baths. In this case, it should has $\left\langle \Delta H_i(0) \Delta H''_j(t) \right\rangle = 0$. As a result, we can calculate $\left\langle \Delta H(0) \Delta H'_j(t) \right\rangle$ by $\left\langle \Delta H(0) \Delta H'_j(t) \right\rangle = \langle \Delta H(0) \Delta H_j(t) \rangle$ and $\langle \Delta H_i(0) \Delta H(0) \rangle$ by $\langle \Delta H_i(0) \Delta H(0) \rangle = \sum_j \langle \Delta H_i(0) \Delta H_j(0) \rangle$. In other word, in studying canonical systems one can apply

$$\rho(r,t) = \frac{\langle \Delta H_i(0) \Delta H_j(t) \rangle}{\langle \Delta H_i(0) \Delta H(0) \rangle} \tag{3}$$

to calculate the PDF of $\Delta H(0)$.

For a microcanonical system, however, the condition $\left\langle \Delta H_i(0) \Delta H''_j(t) \right\rangle = 0$ fails because of

the conservation of the total energy of the system. The conservation of the total energy implies $\sum_j \Delta H_j(t) = 0$, which can be rewritten as $\sum_j [\Delta H'_j(t) + \Delta H''_j(t)] = \Delta H(0) + \sum_j \Delta H''_j(t) = 0$. Multiplying $\Delta H_i(0)$ to the equation one obtains $\sum_j \Delta H_i(0)\Delta H''_j(0) = -\Delta H_i(0)\Delta H(0)$. By calculating the ensemble average it appears as $\sum_j \left\langle \Delta H_i(0)\Delta H''_j(t) \right\rangle = -\left\langle \Delta H_i(0)\Delta H(0) \right\rangle$. Suppose that the lattice includes N particles. Because the nonvanishing correlation $\left\langle \Delta H_i(0)\Delta H''_j(t) \right\rangle$ is resulted from the conservation of the total energy, it is an intrinsic correlation of the system and should be independent of time. It is reasonable to assume that $\left\langle \Delta H_i(0)\Delta H''_j(t) \right\rangle$ should have identical value for each particle. One then derives

$$\left\langle \Delta H_i(0)\Delta H''_j(t) \right\rangle = -\frac{1}{N} \left\langle \Delta H_i(0)\Delta H(0) \right\rangle .$$

Notice that $\Delta H'_j(t) = \Delta H_j(t) - \Delta H''_j(t)$, the PDF of the energy diffusion in a microcanonical system appears as

$$\rho(r,t) = \frac{\langle \Delta H_i(0)\Delta H_j(t) \rangle}{\langle \Delta H_i(0)\Delta H(0) \rangle} + \frac{1}{N}. \tag{4}$$

These two equations 3 and 4 trustily represent the definition equation 2 since one can check that the $\rho(r,t)$ obtained by them satisfy the conditions $\int \rho(r,t)dx = 1$ and $\rho(r,t) \geqslant 0$. In Fig. 1(b) and 1(c), we show the $\rho(r,t)$ calculated by the FC method using canonical ensembles. One can see that for either the FPU$-\beta$ model or the lattice ϕ^4 model the condition $\rho(r,t) \geqslant 0$ is satisfied within numerical errors. In Fig. 3, we show $\int \rho(r,t)dx$ as a function of time for the two models at $T = 0.5$, which indicates that $\int \rho(r,t)dx = 1$ is also satisfied with high precision.

To obtain an isolated system with given temperature, we heat the model to the stationary state with the expected temperature and then take away the heat bath. Applying such a microcanonical system to calculate the PDF, one should employ the eq. 4 instead of the eq. 3. In Fig. 1(d), the dotted line shows the $\rho(r,t)$ calculated by eq. 4 while the solid line shows that of calculated by eq. 3 in the case of the isolated FPU$-\beta$ model. It can be seen that the condition $\rho(r,t) \geqslant 0$ is well satisfied in the former case while fails in the latter case. The condition $\int \rho(r,t)dx = 1$ is also satisfied within numerical errors as shown in Fig. 3 in the former case, while it can be checked that $\int \rho(r,t)dx = 0$ in the latter case. Moreover, we have checked that the PDFs obtained with the canonical ensemble and the microcanonical ensemble are identical with each other at the same temperature within numerical errors.

From Fig. 1(b) and 1(c) one can realize that a PDF obtained by the EK method will approach the corresponding PDF obtained by the FC method when the kick energy $\Delta\widetilde{H}_i(0)$ is small enough.

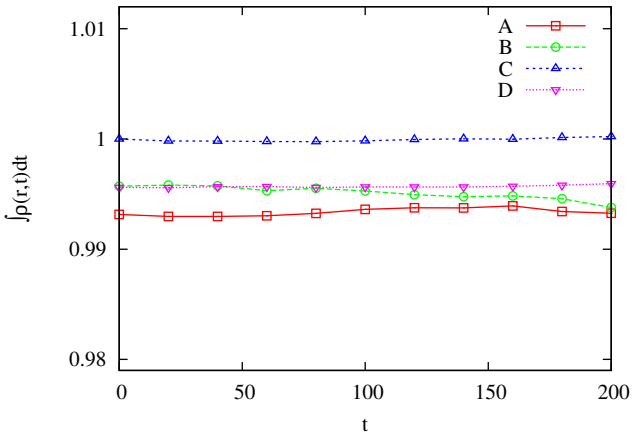

FIG. 3: (color online). $\int \rho(r,t)dr$ *versus* time t for the FPU-β model obtained with canonical ensemble(A) and microcanonical ensemble (B), and the lattice ϕ^4 model with canonical ensemble(C) and microcanonical ensemble (D)

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However, the smaller the kick, the slower the convergence of the PDF. As can be seen in Fig. 1(b), with the same amount of the realizations, the fluctuations of the PDF obtained with the kicks $\Delta\widetilde{H}_i(0) = 5E$ is much larger than that of the PDF obtained with $\Delta\widetilde{H}_i(0) = 10E$. Therefore, decreasing $\Delta\widetilde{H}_i(0)$ needs to dramatically increase the amount of the realizations to achieve a reliable ensemble average.

We now describe the technical details in applying the two methods. Let us take the FPU-β model as an example. For this model, as shown in [21], the two soliton-like packets on the PDF move at a constant velocity, which is supersonic and depends on the temperature of the system. With the dimensionless unit, the soliton-like packets move with $v > 1$. In this case, supposing that the diffusion starts at the middle particle of the lattice and one wants to study the diffusion process up to a time length $t = t_c$, the lattice must have a size $N > 2t_c$ to keep the energy diffusing within the lattice during this period.

To apply the EK method, one may employ a lattice with length $N + 1$ and evolve the system with a sufficiently long time to relax it to a stationary state. Then copy a reference system before adding a kick $\Delta\widetilde{H}_i(0)$ to the middle particle of the lattice. And evolve both the reference system and the kicked system for a time t_c to obtain a set of realization $\Delta\widetilde{H}_j(t)$. This step, i.e., kicking and evolving the two systems, is repeated again and again to obtain the ensemble average $\left\langle \Delta\widetilde{H}_j(t) \right\rangle$. Each round of repeat contributes one realization to the ensemble. In this way, evolving a couple

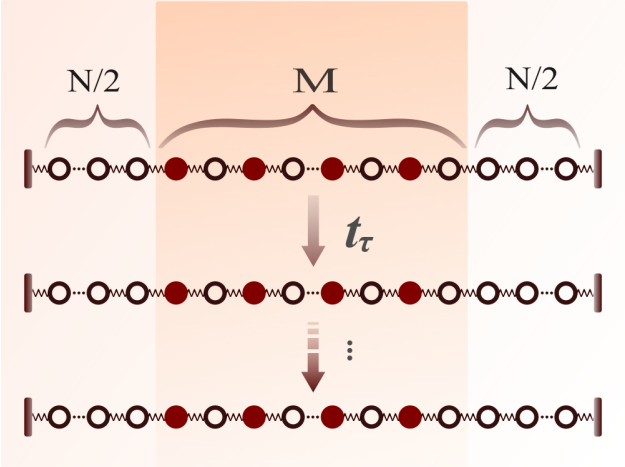

FIG. 4: (color online). Illustration of the strategy of the FC method for calculating the ensemble average. Each of the black particles is applied as independent source where the diffusion is starting at.

of systems for a period t one obtains t/t_c realizations to the ensemble.

To apply the FC method, we apply a lattice with a size $N/2 + M + N/2$, and select M/ξ_τ particles in the middle segment as the sources that the diffusion starts, as illustrated in Fig. 4. Here ξ_τ is a constant which should be sufficiently bigger than the spatial correlation length between particles. For the FPU-β model, one can set $\xi_\tau = 1$ since Fig. 2(a) has indicated that there is no spatial correlations between different particles. For the lattice ϕ^4 model, Fig. 2(c) has shown that the correlation of a particle with its next nearest neighbors has closely approached zero and one can set $\xi_\tau = 3$. In this way, each selected particle can be considered as an independent source and contributes realizations to the ensemble average independently. Based on the same principle, for each of the selected particles, one can further apply a set of continuous records, $\Delta H_i(0)$, $\Delta H_i(t_\tau)$, $\Delta H_i(2t_\tau)$, $\Delta H_i(3t_\tau)$,$\cdots$, as the independent sources, where t_τ is a constant which should be sufficiently bigger than the autocorrelation length of the particle. For the FPU-β and the ϕ^4 models, it can be easily checked that one can apply $t_\tau = 2$ and $t_\tau = 3$ respectively. In this way, each solid circle in Fig. 4 is applied as an independent source of energy diffusion, and contributes a realization to the ensemble.

In this way, by evolving the lattice with a time t one can obtain $M(t - t_c)/\xi_\tau t_\tau$ realizations to the ensemble, which is about $Mt_c/\xi_\tau t_\tau$ times of those obtained in the case of the EK method if $t \gg t_c$.

In the FPU-β model with temperature $T = 0.5$, for example, the soliton-like packets on the PDF move with a velocity $v \sim 1.3$. To investigate the diffusion process extended to $t_c = 1000$,

one can employ a lattice with $N = 3001$ when applying the EK method and apply the middle particle as the source that the energy starts to diffuse. While applying the FC method, one may employ a lattice with 4000 particles and selects the source particles from the middle segment with $M = 1000$. In both cases, the energy diffusion remains within the lattices during the period t_c, since within this time the soliton-like packets can spread over about 1300 particles. Evolving the two lattices with the same time t, the realizations to the ensemble obtained by the FC method is about $Mt_c/\xi_\tau t_\tau \sim 5 \times 10^5$ times of the realizations obtained by the EK method.

Figure 5 (a) shows the PDFs of the FPU-β model at $t_c = 800$ calculated by averages over 3×10^9 and 3×10^{11} realizations respectively. It can be seen that the fluctuations of the PDF are suppressed to a reasonable level in the latter case while is still remarkable in the former case. Even using the FC method, to obtain 3×10^{11} realizations for such a long time diffusion processes is still a hard task for serious computation, to say nothing of the EK method. Fortunately, we achieved the goal by parallel computations using 28 CPUs with half a month. If one wants to obtain the same amount of realizations by the EK method, he must use about 5×10^6 CPUs with the same computation time.

Achieving a sufficiently long diffusion time is necessary to avoid the finite-time effect. The finite-time effect can be ignored for the lattice ϕ^4 model, in which the exponent α tends to $\alpha = 1$ within $t_c < 100$. For other types of lattices with anomalous energy diffusion, such as the FPU-β model and the quartic-FPU model, the finite-time effect is remarkable. The quartic-FPU model represents the unharmonic (or high-temperature) limit of the FPU-β model. As pointed in [33], the qualitative statistical property of this model is temperature-independent because of the scaling behavior. In other words, systems with different temperatures can be scaled together by a proper scaling transformation.

As shown in Fig. 5(a), the PDFs of the energy diffusion for the two models are qualitatively similar with each other, though the soliton-like packets on the PDF of the quartic-FPU model are obviously smaller than that of the FPU-β model. In Fig. 5(b), we plot the $\langle r^2(t) \rangle$ as a function of time with the log-log scale for the two models. Roughly, it seems that both models show a power-law relationship between $\langle r^2(t) \rangle$ and t. To explore the finite-time effect, we plot α by sectional fitting, as Fig. 6(c) shown. In the plot, each point of α is obtained by fitting 4 data points, i.e., it represents the result in a time interval $\Delta t = 200$ correspondingly. One can see that α changes with time initially and converges gradually to a constant, and the finite-time-dependent behavior of α for the two models have different features. It can be seen also that α approaches 1.41 at $t_c > 600$

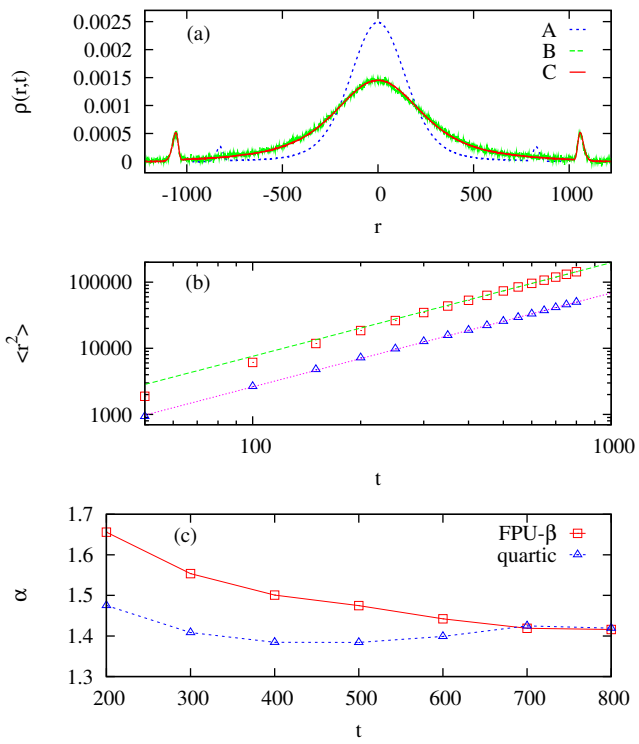

FIG. 5: (color online). The finite-time effect of the diffusion exponent α. (a) The PDFs at $t = 800$: A, for the quartic-FPU model averaged over 6×10^{11} realizations; B and C, for the FPU-β model averaged over 3×10^9 and and 3×10^{11} realizations respectively. (b) The log-log scale plot of $\langle r^2(t) \rangle$ against t for the two models. (c)The time-dependent effect of α for the two models. In both (b) and (c), the squares represent the results of the FPU-β model and the triangles are for the quartic-FPU model.

for both models. This result tends to support the relationship equation of α and β presented in Ref. [18]. However, we still can not sure whether the diffusion exponents have converged exactly at $t_c = 800$. To check it one needs to extend the computation to a longer diffusion time, which already exceeds the capability of our computer system. At least, this fact reminds one to be careful in checking the relationship between α and β by numerical calculations. Instead of studying the diffusion process with the time scale of $t_c \sim 100$ as done by some previous researchers, a diffusion time $t_c > 700$ at least is needed to avoid the finite-time effect.

According to the above results, it seems that the PDFs obtained by the two methods are always symmetric and have only quantitative differences. The symmetric PDFs obtained by the FC method represent the intrinsic behavior of the inner energy. Any part of energy must moves in symmetric way statistically, otherwise the equilibrium can not be maintained. However, the sym-

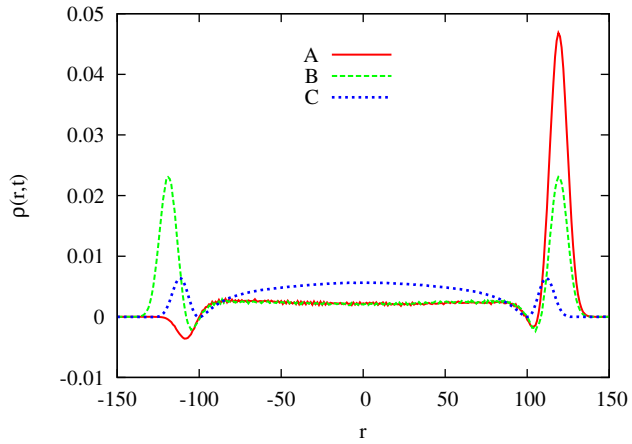

FIG. 6: (color online). The PDFs of the Toda model at $T = 0.5$ and $t = 100$: A, by the EK method with positive kicks; B, by the EK method using the same number of positive and negative kicks; C by the FC method.

metric PDFs obtained by the EK method are particular characteristic of a class of special lattices. By reconsidering the models discussed above, one can find that they have a common feature, i.e., the interaction potential in these models are symmetric. As a consequence, the kick energy added on a particle, either with positive or negative momentum, will be equally transported to the opposite directions. In these lattices, the PDFs obtained by the EK method are always symmetric. On the contrary, for lattices with asymmetric interaction potentials, the PDF obtained by the EK method depends on the way of the kicks. A typical model with asymmetric interaction potential is the Toda model. Figure 6 shows the PDFs computed by the FC and the EK methods respectively for this model in equilibrium with $T = 0.5$. Physically, the inner energy must have equal probability to move to both sides to maintain the equilibrium, the PDF should be symmetric. The figure indicates that the FC method explores this feature correctly. To applying the EK method, we add the kicks in two ways. One is to always add kicks with positive momenta. Notice the asymmetric feature of the interaction potential in this model, a kick with positive momentum will transport more energy to the r.h.s than to the l.h.s. As a result, the PDF of the kick energy should be asymmetric, which is confirmed by the figure. Another way is to add positive and negative kicks with equal probability. In this case, one can obtain a symmetric PDF as the figure shows. Thus, the PDF of the kick energy depends on the way of the kicks. Furthermore, the figure explores another serious problem of the EK method. While the condition $\rho(r,t) \geqslant 0$ well-satisfied for the PDF obtained by the FC method, it fails for the EK method in certain intervals, and thus fails to be a

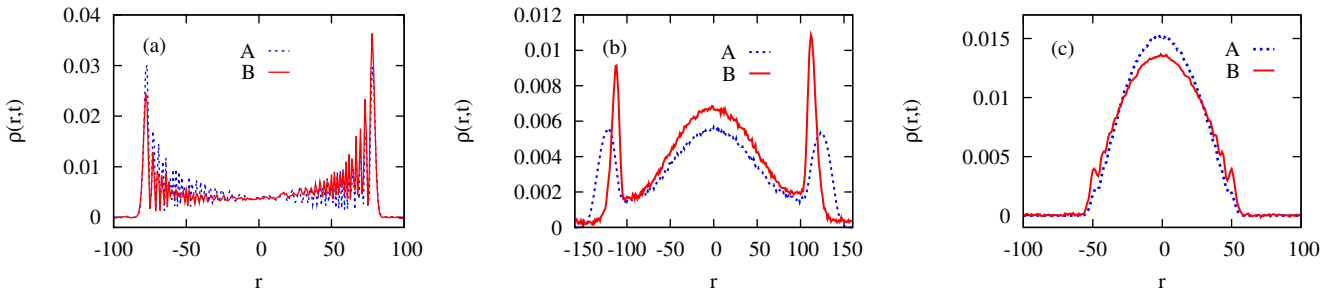

FIG. 7: (color online). The PDFs at $t = 80$ calculated in the case of stationary noequilibrium systems by the EK method (A) and the FC method (B). (a) The harmonic model. (b) The FPU-β model. (c) The lattice ϕ^4 model. In each model, the lattice size is $N = 501$ and the temperatures of the heat baths are fixed at $T_+ = 1$ and $T_- = 0.5$.

probabilistic density function. Therefore, for this model, the EK method is indeed unsuitable for studying the diffusion process.

III. ENERGY DIFFUSION IN NONEQUILIBRIUM LATTICES

Studying the diffusion in stationary nonequilibrium lattices provides us more clear examples to reveal the different diffusion behavior of the inner energy and the kick energy. When coupled with two heat baths with different temperatures, a lattice will approach a nonequilibrium stationary state after a relaxation process. A constant heat flux is then established along the lattice. In such a nonequilibrium lattice, the temperature as well as the average energy can only be defined locally, i.e., $T_i = \langle p_i^2 \rangle$, and $E_i = \langle H_i \rangle$. The $\Delta H_i(0) = H_i(0) - E_i$ depends also on the position of the particles, and, therefore, the energy diffusion starting at different particles may not be statistically identical. In this situation, we study the diffusion starting at the middle particle of a lattice as the illustrating example. Consequently, in a nonequilibrium lattice, one can no longer employ a segment with M particles to calculate the ensemble average, as doing in the case of equilibrium systems. However, the FC method still has the technique advantage in calculating the ensemble average since along the time axis the strategy described in Fig. 4 is still available.

In Fig. 7, we show the PDFs obtained by the EK method (dotted lines) and the FC method (solid lines) for the harmonic model, the FPU-β model and the lattice ϕ^4 model. The temperature of the heat bath in the l.h.s is $T_+ = 1$ and is $T_- = 0.5$ in the r.h.s. Each lattice includes $N = 501$ particles and the diffusion time is $t = 80$. It can be seen that except of the ϕ^4 model, the PDFs

obtained by the EK method are symmetric while those by the FC method are asymmetric. In more detail, it can be checked that $\sigma \simeq 1$ for the PDFs obtained by the EK method. For the PDFs obtained by the FC method, it has $\sigma \simeq 1.4$ for the harmonic model, $\sigma \simeq 1.1$ for the FPU-β model, and $\sigma \simeq 1$ for the lattice ϕ^4 model.

The PDFs with $\sigma \simeq 1$ obtained by the EK method represent the diffusion behavior of the kick energy. As has been pointed out in the end of last section, for lattices with symmetric interaction potentials the kick energy is transported to the opposite directions equally. Either in equilibrium or in nonequilibrium, the environment around the middle particle is similar locally, and thus the kick energy is divided into two equal parts for this type of lattice. The two parts of energy are transported towards the opposite directions hereafter.

The FC method correctly explores the diffusion behavior of the inner energy. The harmonic model is the only one been solved rigidly for the heat conduction problem [7]. The mechanism of the heat transport in this model is clear, i.e., the energy delivered by one heat bath will be transported to the opposite side directly since there is no interaction among normal modes (phonons) in this model. As a result, the energy fluctuation $\Delta H_i(0)$ at the middle particle can be exactly divided into two parts $\Delta H_i(0) = \Delta H_i^+(0) + \Delta H_i^-(0)$. The part $\Delta H_i^+(0)$ comes from the l.h.s heat bath and will move to the r.h.s, and the part $\Delta H_i^-(0)$ comes from the r.h.s heat bath and will move to the l.h.s. In the case of $T_+ = T_-$, it has $\Delta H_i^+(0) = \Delta H_i^-(0)$ and in a later time the amount of the energy $\Delta H_i(0)$ transported to both sides of the middle particle will be the same. While in the case of $T_+ > T_-$, it has $\Delta H_i^+(0) > \Delta H_i^-(0)$ and in a later time the energy moves to the left will be more than that moves to the right. This is the expected diffusion property of the inner energy in this lattice. We define a parameter σ as

$$\sigma \equiv \frac{\int_0^\infty \rho(r,t)dx}{\int_{-\infty}^0 \rho(r,t)dx}$$

to measure the rate of the energy spreading to the two sides of the middle particle. When applying the FC method, it is easy to obtain $\sigma = \frac{\left\langle \Delta H_i(0)\Delta H_i^+(0)\right\rangle}{\left\langle \Delta H_i(0)\Delta H_i^-(0)\right\rangle}$. One thus derives $\sigma = 1$ in equilibrium lattices and $\sigma > 1$ in nonequilibrium lattices, since $\Delta H_i^+(0) = \Delta H_i^-(0)$ in the former and $\Delta H_i^+(0) > \Delta H_i^-(0)$ in the latter cases.

In the case of the FPU-β model, as pointed out in [21], the soliton-like packets keep the initial memory of the direction wherever they move. Equivalently, in this model the energy in the soliton-like packets keeps its initial memory of moving direction. As a result, the energy fluctuation $\Delta H_i(0)$ at the middle particle can be divided into three parts, $\Delta H_i(0) = \Delta H_i^+(0) + \Delta H_i^-(0) +$

$\Delta H_i^0(0)$. Here $\Delta H_i^+(0)$ and $\Delta H_i^-(0)$ come from the high- and low-temperature heat baths and still keep the memory of their moving directions; they will travel to the opposite sides. The part $\Delta H_i^0(0)$ represents the no-memory part which has equal probability to move to either direction. Because of $\Delta H_i^+(0) > \Delta H_i^-(0)$, one can still predict $\sigma = \frac{\langle \Delta H_i(0)\Delta H_i^+(0)\rangle + \langle \Delta H_i(0)\Delta H_i^0(0)\rangle}{\langle \Delta H_i(0)\Delta H_i^-(0)\rangle + \langle \Delta H_i(0)\Delta H_i^0(0)\rangle} > 1$.

For the lattice ϕ^4 model, the Gaussian PDF as well as the derived property of $\langle r^2(t)\rangle \sim t^0$ indicates that the energy diffuses in this system normally. Normal diffusion implies a no-memory random walk. The energy starting at any point will loss totally the initial memory of its moving direction. Thus, $\Delta H_i(0)$ at the middle particle has no memory of the heat baths and will diffuse to either side with equal probability. In this case, one should expect $\sigma = 1$ for this model.

IV. SUMMARY AND DISCUSSION

In summary, the FC method reveals the intrinsic diffusion behavior of the energy in the system, while the EK method displays the diffusion behavior of the kick energy. The inner energy and the kick energy may carry different information, and they may diffuse in different ways.

In lattices with normal energy diffusion, such as in the lattice ϕ^4 model, the energy will totally lose the initial memory. In these lattices, the behavior of the kick and the inner energy appear qualitatively similar because both of them will lose the initial information totally. The PDFs obtained by the two methods appear as Gaussian functions, either in equilibrium or in nonequilibrium. However, the results of the two methods are quantitatively different. The PDFs obtained by the EK method depend on the amplitudes of the kick energy, only when the kicks are weak enough can it approach the results of the FC method.

In lattices with anomalous energy diffusion, the energy may keep part of the initial memory. In equilibrium case, the memory informtion about the moving directions included in the inner energy is symmetric, thus the PDFs obtained by the FC method exhibits such symmetry. When the interaction potentials in lattices, such as the harmonic model or the FPU-β model, are symmetric, the kick energy is thus divided into two equal parts, one moves to the right and the other to the left. As a result, the PDFs obtained by the EK method are also symmetric, although they may be quantatively different from those obtained by the FC method. When the interaction potential is asymmetric, such as in the Toda model, however, the kick energy may diffuse asymmetrically, depending on the way how the kicks are added on. Because of the asymmetric potential, a kick to the right, for instance, will transport more energy to the r.h.s than to the l.h.s., and vice versa.

In this kind of lattices, if one adds positive and negative kicks to the particle with equal probability, the PDFs calculated by the EK method are symmetric, otherwise the PDFs must appear asymmetrically.

In nonequilibrium case, the heat baths added on the two ends of a lattice have different temperatures. As a result, the parts of energy keeping the memory of the corresponding heat bathes arrived at the middle particle are different. The PDFs obtained by the FC method are asymmetric and reveal this intrinsic feature of inner enrgy, while the EK method fails to do so because the kick energy keeps no information of memory of the heat bathes.

Besides the solid theoretical basis, the FC method has remarkable technique advantage over the EK method. Because the FC method uses the energy fluctuations of particles in the system, and any independent energy fluctuation can be treated as $\Delta H_i(0)$ to calculate the ensemble average, thus one can obtain a large set of independent realizations to the ensemble by one round of evolution of the system, as illustrated in Fig. 4. This strategy can reduce the computation time dramatically. The adventage becomes quite remarkable when one studies the long-time diffusion behavior. Comparing with the EK method, the time to evolve the system is shortened by at least five orders when one studies a diffusion process extended to $t_c = 1000$. With this strategy, we calculated the diffusion exponents α of the FPU-β model and the quartic-FPU model upto $t = 800$, and observed that the size-effect on α obviously exist till at least $t = 600$. This fact indicates that the α calculated in some previous works by the EK method with the diffusion time upto $t \sim 100$ is questionable.

To apply the FC method, we introduced the formulae for calculating the PDF of energy diffusion available for canonical and micro-canonical ensembles respectively. In the formulae, the conserved quantity being investigated is $\Delta H(0)$ instead of $\Delta H_i(0)$. This is because that in certain models the energy $\Delta H_i(0)$ adheres constantly a part of energy. To guarantee the normalization of $\rho(r,t)$, we have to consider $\Delta H(0)$ as the energy to be studied. Therefore, the first step to apply the FC method is to detect the energy $\Delta H(0)$ adhered to $\Delta H_i(0)$ by checking the correlation $\langle \Delta H_i(0) \Delta H_j(0) \rangle$. The energy $\Delta H(0)$ needs not to be calculated explicitly, but we demand it locating in a small region and positively correlated to $\Delta H_i(0)$. When these conditions are fulfilled, $\Delta H(0)$ is available for probabilistic descriptions and the $\rho(r,t)$ describes the probability of finding $\Delta H(0)$ at position r and time t.

The definition of the PDF for canonical system presented in this paper is slightly different from that presented in the Ref. [21], in which $\Delta H_i(0)$ is directly applied as the conserved quantity to be

studied. This treatment results no problem for certain lattices such as the FPU-β model. In such a lattice, it has $\Delta H(0) = \Delta H_i(0)$ because of $\langle \Delta H_i(0) \Delta H_j(0) \rangle = 0$ for $i \neq j$. For other systems, such as the lattice ϕ^4 model, $\Delta H(0)$ is slightly bigger than $\Delta H_i(0)$. As a result, the $\rho(r,t)$ obtained can not be normalized exactly. With higher precision, we have checked that $\int \rho(r,t)dx \sim 1.07$ for the lattice ϕ^4 model at $T = 0.5$ when applying the previous definition. Because $\int \rho(r,t)dx$ is still time-independent, it will not alter the value of the exponent α. However, as a PDF, normalization is an expected feature. It is thus better to consider $\Delta H(0)$ as the conservated quantity to be studied.

Acknowledgments

This work is supported by the National Natural Science Foundation of China under Grant No. 10775115, National Basic Research Program of China (973 Program) ($2007CB814800$), and NCETXMU of Xiamen University.

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