

Finite-size effects on current correlation functions

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We study why the calculation of current correlation functions (CCFs) still suffers from finite-size effects even when the periodic boundary condition is taken. Two important one-dimensional, momentum-conserving systems are investigated as examples. Intriguingly, it is found that the state of a system recurs in the sense of microcanonical ensemble average, and such recurrence may result in oscillations in CCFs. Meanwhile, we find that the sound mode collisions induce an extra time decay in a current so that its correlation function decays faster (slower) in a smaller (larger) system. Based on these two unveiled mechanisms, a procedure for correctly evaluating the decay rate of a CCF is proposed, with which our analysis suggests that the global energy CCF decays as $\sim t^{-\frac{2}{3}}$ in the diatomic hard-core gas model and in a manner close to $\sim t^{-\frac{1}{2}}$ in the Fermi-Pasta-Ulam- β model.

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I. INTRODUCTION

In principle, theoretical predictions of statistical mechanics only apply in the thermodynamic limit. But in practice the studied systems are always finite and sometimes can be very small, which is particularly the case in nanoscience. Hence finite-size effects should be carefully analyzed and taken into account. Another important situation where finite-size effects must be considered is to probe thermodynamic properties of a system by molecular dynamics simulations. As usually the system size accessible to simulations is small, the simulation results may significantly deviate.

For a physical quantity \mathcal{A} , the current correlation function (CCF) defined as

$$C_{JJ}(t) \equiv \langle J(0)J(t) \rangle \quad (1)$$

plays a crucial role for understanding its transport properties. Here $\langle \cdot \rangle$ denotes the equilibrium thermodynamic average and $J(t)$ is the total current of \mathcal{A} at time t . The time dependence of C_{JJ} reveals how fluctuations of current J relax in the equilibrium state and determines the transport coefficient of \mathcal{A} by the Green-Kubo formula [1]. However, despite numerous efforts, general properties of a CCF are still elusive, especially in low-dimensional, momentum-conserving systems. For example, early hydrodynamic theory predicts that generally a CCF decays in a manner of power law, i.e., $C_{JJ}(t) \sim t^{-\gamma}$, with γ being half of the dimension of the system [2,3], but studies in recent decades suggest that γ may depend on some detailed properties of a system. In order to clarify this point in the one-dimensional (1D) case, various theoretical methods have been developed [4–16] and recent progress [13,14] suggests that γ for the heat current correlation function be $\frac{1}{2}$ and $\frac{2}{3}$, respectively, for systems with symmetric and asymmetric interparticle interactions. As nowadays it is still impracticable to measure a CCF in laboratories, one has to employ numerical simulations to check these theories. Unfortunately, existing numerical results do not agree with each other [15,16], so that a convincing test is unavailable yet. The main reason for the

disagreement is the finite-size effects induced by the boundary condition inevitably involved in the simulations.

Therefore, a key task is to overcome the influence of finite-size effects. For this aim the fixed and the free boundary conditions are not favorable, because strong finite-size effects could result from boundary reflections, manifested as size-dependent oscillations in C_{JJ} with a period of $\frac{2L}{v_s}$, where L and v_s are, respectively, the size and the sound speed of the system [17]. In contrast, the periodic boundary condition seems to be a better choice. It is free of boundary reflections and is believed to be effective to suppress finite-size effects [18]. Now the periodic boundary condition has been extensively adopted in numerical studies [17–25] as a convention. Nevertheless, for momentum-conserving systems, it has been verified that the CCFs numerically obtained with the periodic boundary condition still have a strong dependence on the system size. Two general size-dependent features are: (i) The CCFs in a smaller system decay faster than in a larger one [19–23], and (ii) size-dependent oscillations with a period of $\frac{L}{v_s}$ instead may occur [17,20–25]. The underlying mechanisms of these phenomena have not been understood yet; thus how to avoid their effects to achieve trustable numerical results is still a challenge.

Our aim here is to reveal the mechanisms of these finite-size effects and show how to capture the asymptotic decaying behavior of CCFs accordingly. We will first show that a local current fluctuation may excite two pulslike components traveling oppositely and colliding repeatedly, so that CCFs in a smaller system decays faster due to more frequent collisions. Then we will show that a finite, momentum-conserving system, has a novel recurrence property even in the equilibrium state. This recurrence may have more fundamental implications, but for our aim here we will show that it induces the size-dependent oscillations in CCFs when the current has correlation with the system configuration. Based on these studies, we will finally propose a reliable procedure to obtain CCFs free from these finite-size effects.

II. MODELS AND FEATURES OF CCFs

We consider two paradigmatic 1D models as illustrating examples: the diatomic hard-core gas model [26] and the

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Fermi-Pasta-Ulam- β (FPU- β) model [27], representing 1D fluids and lattices, respectively. We focus on the CCF of the total energy current in this work, though our analyzing method can be applied equally to other currents and quantities. The gas model consists of N hard-core point particles arranged in order with alternative mass m_o for odd-numbered and m_e for even-numbered particles. The particles travel freely except elastic collisions with their nearest neighbors. Without loss of generality, we follow Ref. [21] to adopt $m_o = 1$, $m_e = 3$, and the total energy current definition $J \equiv \sum j_i$, where $j_i \equiv \frac{1}{2} m_i v_i^3$ with m_i (v_i) being the mass (velocity) of the i th particle. The FPU- β model consists of N point particles as well, defined by the Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m_i} + V(x_i - x_{i-1}) \quad (2)$$

with $V(x) = \frac{x^2}{2} + \frac{x^4}{4}$, where x_i is the displacement of the i th particle from its equilibrium position and p_i is its momentum. In this model, all particles are assumed to have a unit mass; i.e., $m_i = 1$, and the energy current is defined as $J \equiv \sum j_i$ with $j_i \equiv \frac{p_i}{m_i} \frac{\partial}{\partial x_i} V(x_{i+1} - x_i)$ [28]. In both models the periodic boundary condition is imposed. The system size L is set to be $L = N$ so that the density of the particle number is unity. In our simulations the initial condition is set randomly but with two restrictions: The average energy per particle is unity and the total momentum of the system is zero. It should be noticed that due to the null total momentum, the energy current is identical to the heat current [15]; hence our discussions on the energy current in the following applies without any distinctions to the heat current.

In Fig. 1 we plot the energy CCF of the two models. The common finite-size effect shared by them is that the smaller the system is, the faster the energy CCF decays. Another finite-size effect is observed only in the gas model, which appears as oscillations whose period depends on the system size.

III. SOUND MODE COLLISIONS

In order to reveal the mechanisms of these finite-size effects, let us first study the spatiotemporal correlation function of local

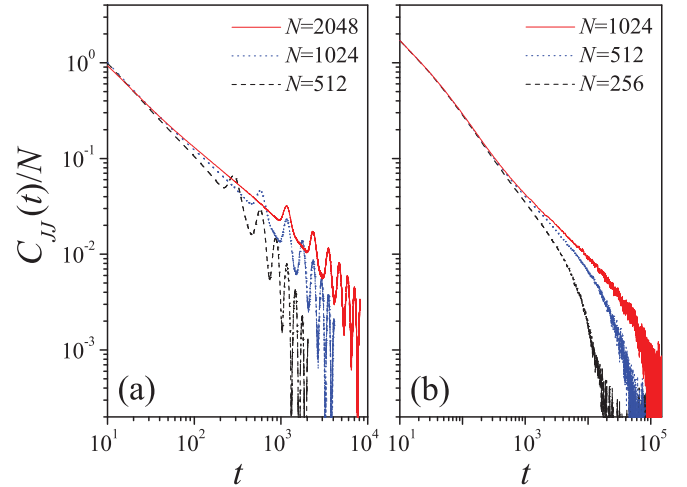


FIG. 1. (Color online) The energy current correlation function for the gas model (a) and the FPU- β model (b). The period of oscillations observed in (a) is measured to be $\frac{L}{v_s}$ (v_s is the sound speed of the system).

energy currents. We divide the system into $\frac{L}{b}$ bins in space of equal width $b = 1$. The local energy current in the k th bin and at time t is defined as $J^{\text{loc}}(x, t) \equiv \sum_i j_i(t)$, where $x \equiv kb$ and the summation is taken over all particles reside in the k th bin at time t . The spatiotemporal correlation function of local currents is defined as [22,23,25,29–31]

$$C(x, t) \equiv \langle J^{\text{loc}}(0, 0) J^{\text{loc}}(x, t) \rangle. \quad (3)$$

Note that $J(t) = \sum_k J^{\text{loc}}(kb, t)$, hence we have $C_{JJ}(t) = \frac{L}{b^2} \int C(x, t) dx$ considering that our systems are homogeneous in space [23]. It has been found that $C(x, t)$ features a pair of pulses moving oppositely away from $x = 0$ at the sound speed [23,29,30], which are recognized to be the hydrodynamic mode of sound.

In Fig. 2 we show $C(x, t)$ at various times for both models. The two peaks representing the sound mode can be clearly identified. Their moving speed is measured to be $v = 1.75$ in the gas model and $v = 1.50$ in the FPU- β model, agreeing with

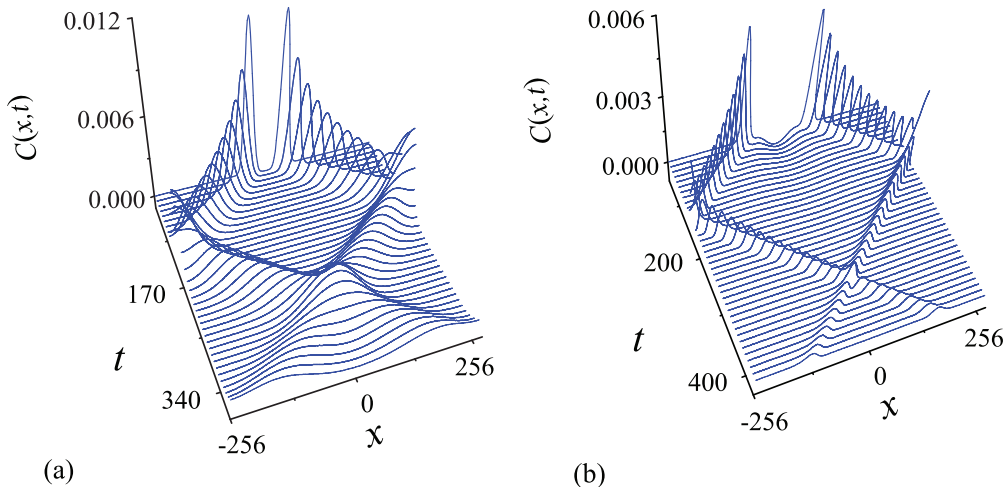


FIG. 2. (Color online) The spatiotemporal correlation function of local energy (heat) currents for the 1D gas model (a) and the FPU- β model (b). The system size is $L = 512$ in both cases.

the sound speed in each system very well. $C(x,t)$ provides more useful information of local currents. As suggested by Fig. 2, a local current, say, at $x = 0$, will excite local currents centered at $x = \pm vt$ after time t . As $C(x,t)$ is positive around $x = \pm vt$, the excited local currents also have the same flowing direction of the original local current. If the system has an infinite size, these excited local currents will never encounter, but in a finite system they will collide with each other repeatedly (see Fig. 2). Unless they do not interact, their collisions will damage the excited local currents and in turn cause the total current J to decay. The collisions take place more frequently in shorter systems, implying that CCFs should decay faster, in good consistence with the result presented in Fig. 1. However, the sound mode collisions can not explain the size-dependent oscillations of $C_{JJ}(t)$ observed in the gas model, because they take place with a period of $\tau_{\text{col}} \equiv \frac{L}{2v_s}$, while $C_{JJ}(t)$ oscillates with the period of $\frac{L}{v_s}$ [see Fig. 1(a)].

IV. RECURRENCE

We find that there is an interesting recurrence in both systems and it is responsible for the oscillations of $C_{JJ}(t)$ in the gas model. Let us denote the state of a system at time t by the vector $\mathbf{r}(t) \equiv [p_1(t), \dots, p_N(t), x_1(t), \dots, x_N(t)]^T$ and study the state correlation function

$$R(t) \equiv \langle \mathbf{r}(0) \cdot \mathbf{r}(t) \rangle \quad (4)$$

to explore the recurrence. The results are shown in Fig. 3: In the sense of ensemble average, both systems recur with a period of $\tau_{\text{rec}} \equiv \frac{L}{v_s}$. In addition, the features of $R(t)$ in the gas model match very well with those of $C_{JJ}(t)$ [see Fig. 3(a) for a comparison], suggesting strongly that the oscillations of $C_{JJ}(t)$ are closely related to the recurrence. Indeed, in the gas model $\langle j_i(t)x_i(t) \rangle = \langle \frac{1}{2}m_i v_i^3 x_i \rangle = 0$ but $\langle j_i(t)p_i(t) \rangle = \langle \frac{1}{2}m_i^2 v_i^4 \rangle = 2e$, where e is the average energy of a particle that has been set to be unity, showing that

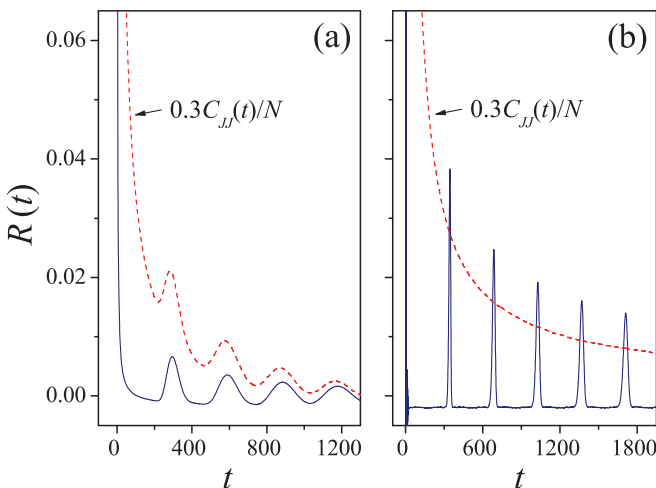


FIG. 3. (Color online) The comparison between the state correlation function $R(t)$ (blue solid line) and the energy current correlation function $C_{JJ}(t)$ (red dashed line) for the gas mode (a) and the FPU- β model (b). In order to have a close comparison, $C_{JJ}(t)$ is shifted down by a factor of $\frac{0.3}{N}$. The system size adopted is $L = 512$ in both panels.

local currents and the system's momentum configuration are definitively correlated. However, this is not the case in the FPU- β model, where it has been numerically checked and verified that not only $\langle j_i(t)x_i(t) \rangle = 0$, but also $\langle j_i(t)p_i(t) \rangle = 0$. This explains why the recurrence does not cause oscillations of $C_{JJ}(t)$ in this model.

V. EVALUATING DECAYING RATES OF CCFs

Based on the analysis of the two finite-size effects, it can be concluded that how a CCF decays in the thermodynamic limit can only be evaluated by extrapolating $C_{JJ}(t)$ in the time range of $t \leq \tau_{\text{col}} = \frac{L}{2v_s}$. Beyond this range, even though the extra decay induced by each sound mode collision may be weak, the cumulative effect of multiple collisions can be significantly large. For $t \leq \tau_{\text{col}}$, if the current has no correlation to the system configuration as in the FPU- β model, the function $C_{JJ}(t)$ calculated with a finite system size L should agree with the true CCF in the thermodynamic limit. Otherwise, as in the case of the gas model, the finite-size effect caused by the recurrence may manifest. But in general, the deviation of $C_{JJ}(t)$ evaluated with a finite system size will decrease as the system size increases.

On the other hand, in order to facilitate the evaluation of the decay rate, a helpful but not necessary trick is to exclude the initial transient stage of $C_{JJ}(t)$ in performing the extrapolation. As there is no theoretical guide yet, the time the transient stage lasts, denoted by t_0 , has to be determined in a practical way. So we suggest the following procedure to obtain the decaying rate, γ , of a CCF: Set a tentative transient time t_0 and measure the decaying rate $\tilde{\gamma}$ as a function of both t_0 and L by best fitting $C_{JJ}(t)$ over the time range of (t_0, τ_{col}) , then study the dependence of $\tilde{\gamma}$ on t_0 and L , and identify γ to be the value of $\tilde{\gamma}$ invariant of further increasing of t_0 and L after certain values. Table I shows the value of $\tilde{\gamma}$ for the energy CCF in both systems; one can find that, as expected, the transient time may affect the convergence rate of $\tilde{\gamma}$ but does not affect the value it tends to. The data presented in Table I give a strong support that the energy CCF decays as $C_{JJ}(t) \sim t^{-\gamma}$ with $\gamma = \frac{2}{3}$ for the gas model. For the FPU- β model, though the decay rate tends to $\frac{1}{2}$ from above monotonously, its value has not converged even when the system size is as large as $L = 65536$. However, it can be anticipated that γ for the FPU- β model is very likely different from $\frac{3}{5}$ as having been constantly concluded in previous numerical studies [15, 19, 29]. As a comparison, in Fig. 4(b) we plot $t^{\gamma^*} C_{JJ}(t)$ with $\gamma^* = \frac{1}{2}$

TABLE I. The decaying rate $\tilde{\gamma}$ of the energy CCF for the two systems measured by the best fitting to $C_{JJ}(t)$ over the time interval of (t_0, τ_{col}) . The relative error of $\tilde{\gamma}$ ranges from 0.3% to 0.6%.

model	system size L				
	4096	8192	16384	32768	65536
gas ($t_0 = 100$)	0.725	0.699	0.683	0.679	0.672
gas ($t_0 = 1000$)	0.762	0.704	0.691	0.681	0.675
FPU- β ($t_0 = 1000$)	0.614	0.608	0.588	0.576	0.525
FPU- β ($t_0 = 2000$)	-	0.548	0.577	0.568	0.517

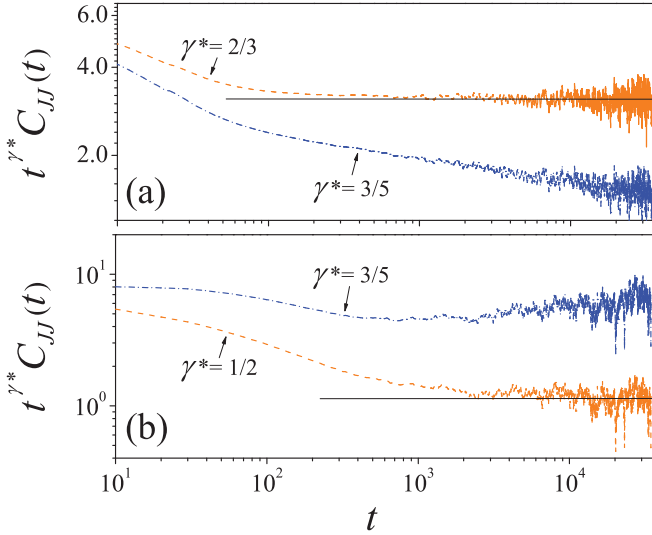


FIG. 4. (Color online) (a) The comparison of the rescaled energy CCF, $t^{\gamma^*} C_{JJ}(t)$, for the gas model with $\gamma^* = \frac{2}{3}$ (orange dashed line) and $\gamma^* = \frac{3}{5}$ (blue dash-dotted line). The black horizontal line is plotted for reference. The system size is $L = 65536$. (b) The same as (a) but for the FPU- β model with $\gamma^* = \frac{3}{5}$ and $\gamma^* = \frac{1}{2}$ instead. The system size is $L = 131072$.

and $\frac{3}{5}$, respectively; their tendency difference can be clearly distinguished.

The study of Table I suggests that only in a very large system (to the simulations) may the stationary asymptotic decaying rate of $C_{JJ}(t)$ be revealed. For example, in order to reach the precision to reliably distinguish which value γ may take among $\frac{1}{2}$, $\frac{3}{5}$, and $\frac{2}{3}$ in the FPU- β model, the system size should be at least about $L = 65536$, which has never been attempted by previous studies. Moreover, in previous studies, without a careful analysis of the finite-size effects, the time range for evaluating γ had to be chosen empirically. This may result in big uncertainty in the results and make it hard to avoid the bias due to existing theoretical predictions or subjective factors.

VI. SUMMARY AND DISCUSSION

To summarize, we have shown that in the equilibrium state, a momentum-conserving system may recur in the sense of

the ensemble average [32] after a size-dependent period of $\tau_{\text{rec}} = \frac{L}{v_s}$. This recurrence may induce oscillations of a CCF if the current is correlated to the system configuration. It also implies long time correlations in the system. We emphasize that unlike the well known Fermi-Pasta-Ulam recurrence [27,33] and the Poincaré recurrence [34], the recurrence found here features the finite size of a system, the equilibrium state, and the ensemble average, hence is distinct from them in nature (e.g., its characteristic recurrence time τ_{rec} is much shorter than that of the FPU and the Poincaré recurrence). Besides the energy CCF, this recurrence should have effects on other quantities as well, as long as they are correlated to the system configuration. For this reason, it would be interesting to figure out the role it plays in any other related statistical and dynamical properties.

In addition, we have shown that the sound mode collisions occurring with a period of $\tau_{\text{col}} = \frac{L}{2v_s}$ can induce extra scattering to currents and this explains why a CCF in a smaller system decays faster. By taking into consideration these findings, we have proposed a procedure for reliably measuring the asymptotic decaying rate of a CCF. Our analysis has suggested that the energy CCF decays as $\sim t^{-\frac{2}{3}}$ in the gas model and in a manner close to $\sim t^{-\frac{1}{2}}$ in the FPU- β model, in agreement with recent theoretical predictions that, in 1D momentum-conserving systems, the energy CCF should decay as $\sim t^{-\frac{2}{3}}$ and $\sim t^{-\frac{1}{2}}$ when the interparticle interactions are asymmetric and symmetric, respectively [13,14]. [Note that the gas (the FPU- β) model belongs to the class of asymmetric (symmetric) interactions.]

Nevertheless, we recall that in 1D momentum-conserving lattices with asymmetric interactions, the heat conductivity may converge and the heat CCF may decay more rapidly [35,36]. This fact implies that there may be some crucial difference between fluid and lattice systems, and the decaying prediction of $\sim t^{-\frac{2}{3}}$ may only apply to fluids. This point should be clarified in future.

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- [1] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II: Nonequilibrium Statistical Mechanics* (Springer, New York, 1991); D. Andrieux and P. Gaspard, *J. Stat. Mech.* (2007) P02006.
 - [2] B. J. Alder and T. E. Wainwright, *Phys. Rev. A* **1**, 18 (1970).
 - [3] M. H. Ernst, E. H. Hauge, and J. M. J. van Leeuwen, *Phys. Rev. Lett.* **25**, 1254 (1970); J. R. Dorfman and E. G. D. Cohen, *ibid.* **25**, 1257 (1970).
 - [4] T. Prosen and D. K. Campbell, *Phys. Rev. Lett.* **84**, 2857 (2000).
 - [5] O. Narayan and S. Ramaswamy, *Phys. Rev. Lett.* **89**, 200601 (2002).
 - [6] S. Lepri, R. Livi, and A. Politi, *Phys. Rev. E* **68**, 067102 (2003).
 - [7] T. Mai and O. Narayan, *Phys. Rev. E* **73**, 061202 (2006).
 - [8] J. S. Wang and B. Li, *Phys. Rev. Lett.* **92**, 074302 (2004).
 - [9] G. Basile, C. Bernardin, and S. Olla, *Phys. Rev. Lett.* **96**, 204303 (2006).
 - [10] A. Pereverzev, *Phys. Rev. E* **68**, 056124 (2003).
 - [11] J. Lukkarinen and H. Spohn, *Commun. Pur. Appl. Math.* **61**, 1753 (2008).
 - [12] G. R. Lee-Dadswell, B. G. Nickel, and C. G. Gray, *Phys. Rev. E* **72**, 031202 (2005); *J. Stat. Phys.* **132**, 1 (2008).
 - [13] L. Delfini, S. Lepri, R. Livi, and A. Politi, *Phys. Rev. E* **73**, 060201 (2006); *J. Stat. Mech.* (2007) P02007.
 - [14] H. van Beijeren, *Phys. Rev. Lett.* **108**, 180601 (2012).
 - [15] S. Lepri, R. Livi, and A. Politi, *Phys. Rep.* **377**, 1 (2003).
 - [16] A. Dhar, *Adv. Phys.* **57**, 457 (2008).

- [17] E. Brunet, B. Derrida, and A. Gerschenfeld, *Europhys. Lett.* **90**, 20004 (2010).
- [18] S. G. Volz and G. Chen, *Phys. Rev. B* **61**, 2651 (2000).
- [19] L. Wang and T. Wang, *Europhys. Lett.* **93**, 54002 (2011).
- [20] A. Dhar, *Phys. Rev. Lett.* **88**, 249401 (2002).
- [21] P. Grassberger, W. Nadler, and L. Yang, *Phys. Rev. Lett.* **89**, 180601 (2002).
- [22] G. Casati and T. Prosen, *Phys. Rev. E* **67**, 015203(R) (2003).
- [23] T. Prosen and D. K. Campbell, *Chaos* **15**, 015117 (2005).
- [24] B. Li, G. Casati, J. Wang, and T. Prosen, *Phys. Rev. Lett.* **92**, 254301 (2004).
- [25] V. A. Levashov, J. R. Morris, and T. Egami, *Phys. Rev. Lett.* **106**, 115703 (2011).
- [26] G. Casati, *Found. Phys.* **16**, 51 (1986).
- [27] E. Fermi, J. Pasta, and S. Ulam, Report No. LA-1940, 1955 (unpublished), reprinted in E. Fermi, *Collected Papers* (University of Chicago Press, Chicago, 1965), Vol. II, p. 978.
- [28] T. Mai, A. Dhar, and O. Narayan, *Phys. Rev. Lett.* **98**, 184301 (2007).
- [29] S. Lepri, R. Livi, and A. Politi, *Europhys. Lett.* **43**, 271 (1998).
- [30] S. Chen, Y. Zhang, J. Wang, and H. Zhao, *Phys. Rev. E* **87**, 032153 (2013).
- [31] H. Zhao, *Phys. Rev. Lett.* **96**, 140602 (2006).
- [32] We have checked and found that in momentum nonconserving systems, such as the ϕ^4 lattice, such recurrence does not occur.
- [33] Focus issue: The Fermi-Pasta-Ulam problem-the first 50 years, D. K. Campbell, P. Rosenau, and G. M. Zaslavsky, *Chaos* **15**, 015101 (2005).
- [34] A. Wintner, *The Analytical Foundations of Celestial Mechanics* (Princeton University Press, Princeton, 1947), p. 90.
- [35] Y. Zhong, Y. Zhang, J. Wang, and H. Zhao, *Phys. Rev. E* **85**, 060102(R) (2012).
- [36] S. Chen, Y. Zhang, J. Wang, and H. Zhao, [arXiv:1204.5933](https://arxiv.org/abs/1204.5933).