

Energy relaxation in disordered lattice φ^4 system: The combined effects of disorder and nonlinearity

Jianjin Wang(汪剑津), Yong Zhang(张勇), and Daxing Xiong(熊大兴)
Citation: Chin. Phys. B, 2020, 29 (**12**): 120503. DOI: 10.1088/1674-1056/abc15b
Journal homepage: http://cpb.iphy.ac.cn; http://iopscience.iop.org/cpb

What follows is a list of articles you may be interested in

Directed transport of coupled Brownian motors in a two-dimensional traveling-wave potential

Wei-Xia Wu(吴魏霞), Zhi-Gang Zheng(郑志刚), Yan-Li Song(宋艳丽), Ying-Rong Han(韩英荣), Zhi-Cheng Sun(孙志成), Chen-Pu Li(李晨璞)
Chin. Phys. B, 2020, 29 (**9**): 090503. DOI: 10.1088/1674-1056/ab99b7

Existence of spontaneous symmetry breaking in two-lane totally asymmetric simple exclusion processes with an intersection

Bo Tian(田波), Ping Xia(夏萍), Li Liu(刘莉), Meng-Ran Wu(吴蒙然), Shu-Yong Guo(郭树勇)
Chin. Phys. B, 2020, 29 (**5**): 050505. DOI: 10.1088/1674-1056/ab820e

Energy relaxation in disordered lattice φ^4 system: The combined effects of disorder and nonlinearity

Jianjin Wang(汪剑津), Yong Zhang(张勇), and Daxing Xiong(熊大兴)
Chin. Phys. B, 2020, 29 (**12**): 120503. DOI: 10.1088/1674-1056/abc15b

One-dimensional mass transport with dynamic external potentials

Xingxing Zhang(张星星), Dongqin Zheng(郑冬琴), Weirong Zhong(钟伟荣)
Chin. Phys. B, 2019, 28 (**2**): 020505. DOI: 10.1088/1674-1056/28/2/020505

Transport dynamics of an interacting binary Bose–Einstein condensate in an incommensurate optical lattice

Cui Guo-Dong, Sun Jian-Fang, Jiang Bo-Nan, Qian Jun, Wang Yu-Zhu
Chin. Phys. B, 2013, 22 (**10**): 100501. DOI: 10.1088/1674-1056/22/10/100501

Energy relaxation in disordered lattice ϕ^4 system: The combined effects of disorder and nonlinearity*

Jianjin Wang(汪剑津)[1], Yong Zhang(张勇)[2], and Daxing Xiong(熊大兴)[3,†]

[1] Department of Physics, Jiangxi Science and Technology Normal University, Nanchang 330013, China
[2] Department of Physics, Xiamen University, Xiamen 361005, China
[3] School of Science, Jimei University, Xiamen 361021, China

(Received 11 August 2020; revised manuscript received 22 September 2020; accepted manuscript online 15 October 2020)

We address the issue of how disorder together with nonlinearity affect energy relaxation in the lattice ϕ^4 system. The absence of nonlinearity leads such a model to only supporting fully localized Anderson modes whose energies will not relax. However, through exploring the time decay behavior of each Anderson mode's energy–energy correlation, we find that adding nonlinearity, three distinct relaxation details can occur. (i) A small amount of nonlinearity causes a rapid exponential decay of the correlation for all modes. (ii) In the intermediate value of nonlinearity, this exponential decay will turn to power-law with a large scaling exponent close to -1. (iii) Finally, all Anderson modes' energies decay in a power-law manner but with a quite small exponent, indicating a slow long-time tail decay. Obviously, the last two relaxation details support a new localization mechanism. As an application, we show that these are relevant to the nonmonotonous nonlinearity dependence of thermal conductivity. Our results thus provide new information for understanding the combined effects of disorder and nonlinearity on energy relaxation.

Keywords: classical transport, localized modes, Anderson localization

PACS: 05.60.Cd, 63.20.Pw, 66.70.−f **DOI:** 10.1088/1674-1056/abc15b

1. Introduction

Over the past decades, the study of energy relaxation in anharmonic disordered systems has attracted a lot of interest both theoretically[1–12] and experimentally.[13–18] In a simple case of harmonic disordered systems, this is relevant to the celebrated Anderson localization phenomenon predicted for noninteracting electrons propagating in uncorrelated random landscapes,[19] which has the strongest effect in one dimension. In such a case, all the linear eigenmodes, i.e., the Anderson modes are localized, which means that any initially localized wave packet will remain localized for all time. Therefore, there is no energy relaxation at all. However, whenever the nonlinearities are added to such linear disordered models, these Anderson modes can interact with each other and result in more complex situations. Hence, transport in systems with combined effects of disorder and nonlinearity is currently still an open question of fundamental interest.

Due to these complicated situations, numerical studies are very favorable for studying such issues. So far two kinds of numerical approaches have been widely employed to detect energy relaxation in these systems. The first one called the wave packet dynamics is often applied to study the systems of zero temperature.[6,8,10] In this method, some amounts of energy are initially endowed to one or several sites of the system and one then monitors the spreading process of these energy wave pockets. In this respect, most studies were focused on two typical disordered anharmonic Klein–Gordon (KG) and discrete nonlinear Schrödinger (DNLS) models[6] and it has been shown that the energy wave packets in these systems under the combined effects of disorder and nonlinearity always spread out subdiffusively. The underlying mechanisms are related to the relevant systems' chaotic dynamics, i.e., the spatiotemporal fluctuations of the chaotic seeds inside the wave packet.[6,8,10]

In the case of finite-temperature systems, the relevant physics and underlying pictures are richer. One has to adopt longer molecular dynamics simulations to obtain the information of energy relaxation. With the usual nonequilibrium method, i.e., adding two thermal baths to two ends of the one-dimensional (1D) anharmonic disorder Fermi–Pasta–Ulam (FPU) systems, earlier studies have revealed that there is a transition from normal transport following the Fourier law at lower temperatures to anomalous non-Fourier transport at high temperatures.[20] Nevertheless, this claim has been argued later by observing that adding only a small amount of nonlinearity is already sufficient to lead to the normal heat conduction and thus there is no evidence for the claimed temperature-dependent transition.[21] Recently, this normal transport behavior has been further verified by using the equilibrium correlation method to explore the relaxation process of local energy

*Project supported by the National Natural Science Foundation of China (Grant Nos. 11847015, 11975190, 11575046, and 11964012), the Natural Science Foundation of Fujian Province, China (Grant No. 2017J06002), and the Start-up Fund from Jiangxi Science and Technology Normal University (Grant No. 2017BSD002).

†Corresponding author. E-mail: xmuxdx@163.com

© 2020 Chinese Physical Society and IOP Publishing Ltd

fluctuations. By studying the equilibrium energy–energy correlation functions that represents the spatial probability density function (PDF) of energy spreading, one found that the time-dependent mean squared displacement of this PDF follows the usual scaling of normal transport, but the PDF is an unusual non-Gaussian function, which shows a first example of non-Gaussian normal energy diffusion in many-body systems.[22]

The non-Gaussian normal diffusion observed in the finite-temperature anharmonic disordered systems implies that compared to the knowledge of subdiffusion shown in the counterpart zero-temperature systems, there are still much interesting details that need to explore. Motivated by this, in the present paper we study the relaxation of single Anderson mode's energy to fill some of the gaps. Toward that end we employ the time decay of single Anderson mode's energy–energy equilibrium autocorrelation with the increase of the nonlinearity to capture such relaxation details. Our main finding is that while for a small amount of nonlinearity this correlation for the Anderson modes decays in a quite rapid exponential manner, in the case of large nonlinearity this decay becomes slow and shows a power-law long-time tail, first from the modes of a lower wave number. This implies that even adding a small amount of nonlinearity is already sufficient to cause the delocalization of the Anderson modes, whereas further increasing nonlinearity can otherwise result in new localization mechanisms. Our results thus provide new information for understanding the combined effects of disorder and nonlinearity on transport.

2. Model

We consider a 1D disordered lattice ϕ^4 system with Hamiltonian

$$H=\sum_{i=1}^{N}\frac{m_i v_i^2}{2}+V(x_{i+1}-x_i)+U(x_i), \tag{1}$$

where N is the total number of particles and is equivalent to the system size; m_i, v_i, and x_i are, respectively, the i-th particle's mass, velocity, and displacement from the equilibrium position. $V(x_{i+1}-x_i)=(x_{i+1}-x_i)^2/2$ is the harmonic interparticle potential and $U(x_i)=k_0x_i^2/2+\lambda x_i^4/4$ is the on-site potential. The property of disorder here is introduced by choosing m_i randomly from a uniform distribution in an interval $[0.8,1.2]$. The strength of nonlinearity is represented by λ.

We note that with an appropriate setup, this system's linear counterpart, i.e., the case with $\lambda=0$ and that only the effect of disorder is considered, can support fully localized Anderson modes. This is distinct from the system without including the on-site potential $[U(x_i)=0]$, whose low-frequency Anderson modes instead remain extended.[21] Our setup for obtaining the fully localized Anderson modes is achieved by adjusting k_0, i.e., the strength of the linear term in $U(x_i)$, suitably, with respect to a fixed finite system size N. We have verified that with the Thouless criterion and through studies of system's energy relaxation process, as long as $k_0\geq 1$, the system's localization length is always less than 3000.[22] Thus, in the following we fix $k_0=1$ and $N=4096$.

3. The fully localized Anderson modes

To see the property of localization, we first give each Anderson mode's localization length. In Fig. 1(a) we plot the ratio ξ/N of the localization length ξ with respect to the system length N as a function of mode's index (wave number) k. Here, k is proportional to the mode's frequency as shown in Fig. 1(b). It should be noted that ξ is inversely proportional to the degree of mode's localization[23] as a mode owning a smaller localization length implies higher localization. In practice, ξ can be either computed by the transfer matrix method[23,24] or through measuring the spatial correlation of mode's kinetic energy in the equilibrium state,[25] here we use the first approach. As can be seen in Fig. 1(a), the curve of ξ/N vs. k shows a arcuation shape, i.e., the Anderson modes with a middle value of k have a relatively large ξ compared to

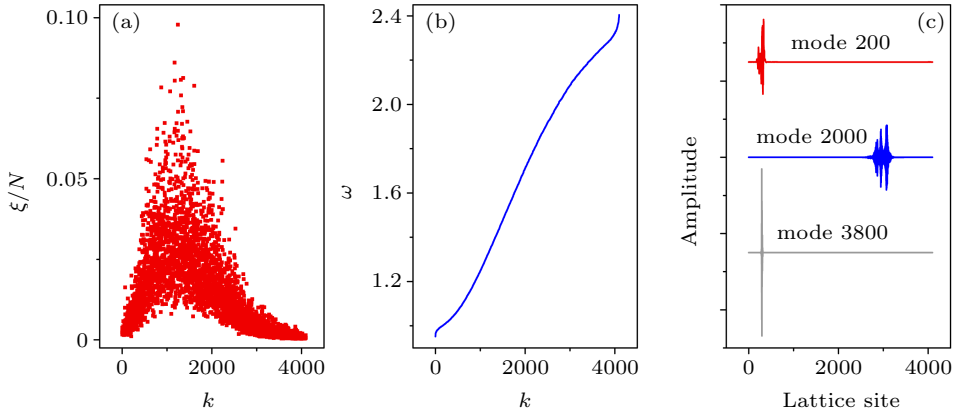


Fig. 1. The fully localized Anderson modes. (a) The ratio of mode's localization length ξ with respect to the system length N vs. mode's index k; (b) mode's frequency ω vs. k, (c) profiles of three representative Anderson modes. Here, for convenient identification of each mode, we shift their amplitudes along the vertical axis.

the modes with k in both ends. In addition, the maximum of ξ/N is only about 0.1, suggesting that all the Anderson modes' localization lengths are certainly much smaller than N. As examples, figure 1(c) shows profiles of three representative Anderson modes, i.e., the 200th, 2000th, and 3800th modes. These confirm the full localization properties of the modes.

4. Relaxation: single Anderson mode's energy–energy autocorrelation

As mentioned, by adding nonlinearities the Anderson modes which are initially localized will interact with each other and this interaction gives rise to more complex situations. To capture some of the aspects of these complicated situations, we study the time evolution of the equilibrium single Anderson mode's energy–energy autocorrelation, defined by

$$C_{ee}^{k}(t)=\frac{\langle \Delta e_k(t)\Delta e_k(0)\rangle}{\langle \Delta e_k(0)\Delta e_k(0)\rangle}, \tag{2}$$

where $e_k(t)$ is the instantaneous energy of the Anderson mode k and $\Delta e_k(t)=e_k(t)-\langle e\rangle$ with $\langle\cdot\rangle$ denoting the ensemble average. $e_k(t)$ for each Anderson mode is evaluated through the following projection method.[26] We first prepare an equilibrium state of temperature $T=1.5$. This is done by connecting the two ends of the system to two thermal bathes with the set temperature for a long enough time. After the system has been relaxed to this equilibrium state showing evidence that all particles' velocities follow a Gaussian distribution pointing to the given temperature, we then remove the thermal baths (Noose–Hoover or Langevin, see also below) and set $x_l=\frac{u_l}{\sqrt{m_l}}\exp(-\mathrm{i}\omega t)$, which enables us to linearize the motion equation of particles and so that the dynamic matrix can be diagonalized. Let $\boldsymbol{V}^k$ and ω_k be the k-th normalized eigenvector and eigenvalue of the dynamic matrix, the projection of the motion onto the k-th Anderson mode is $Q_k(t)=\sum_{j=1}^{N}\sqrt{m_j}x_j(t)V_j^k$ and $P_k(t)=\sum_{j=1}^{N}\sqrt{m_j}v_j(t)V_j^k$ with $k=1,\ldots,N$, and finally $e_k(t)=(P_k^2+\omega_k^2Q_k^2)/2$ can be obtained. With this normal mode energy, $C_{ee}^{k}(t)$ is measured by performing simulations from different sets of randomly assigned initial conditions for the average. For this and below we adopt the Runge–Kutta algorithm of the 7–8th order with a time step $\delta t=0.01$ to integrate the Hamiltonian equations

$$\dot{x}_i=\frac{\partial H}{\partial p_i},\quad \dot{p}_i=-\frac{\partial H}{\partial x_i}. \tag{3}$$

We use a total ensemble of size 8×10^8 for the average.

Figure 2 shows $C_{ee}^{k}(t)$ for three representative modes $k=200$, 2000, and 3800 for $\lambda=0.03$, 0.1, and 1, respectively. For clearly clarifying the relevant details with the increase of nonlinearity for each mode, figures 2(a)–2(c) present the results for fixed number of mode and figures 2(d)–2(f) give the results for fixed λ. As can be seen, as long as adding a small amount of nonlinearity ($\lambda=0.03$), $C_{ee}^{k}(t)$ for all Anderson modes decays exponentially with time t, indicating a rapid delocalization process [see Fig. 2(d)]. This is in contrast to the fully localized behavior observed in the relevant linear model where not any delocalization will be shown, but consistent with the observed normal thermal conduction satisfying Fourier's law conjectured in Ref. [21]. In addition, from Fig. 2(c) and combining the result of Fig. 1(a) one also infers that in this small amount of nonlinearity case, $C_{ee}^{k}(t)$ for the mode with a relatively long localization length ($k=2000$ for example) generally decays more rapid than other modes ($k=200,3800$). This might imply the general property of delocalization for Anderson modes with weak nonlinearity.

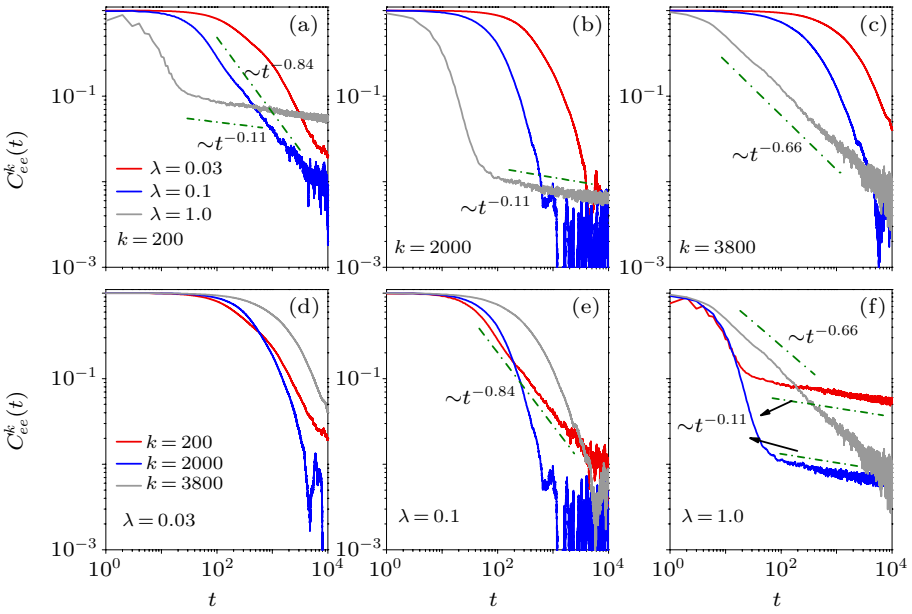


Fig. 2. Single Anderson mode relaxation represented by $C_{ee}^{k}(t)$ for $\lambda=0.03$, 0.1, and 1, respectively. Here we present three representative modes of $k=200$, 2000, and 3800 for examples.

With the increase of nonlinearity, more complex situations with rich details of relaxation occur. In the intermediate value of nonlinearity ($\lambda = 0.1$), $C_{ee}^{200}(t)$ in a long time first turns from the conventional exponential time decay to a power-law time decay t^{μ} with a large exponent of $\mu \simeq 0.84$ [see Fig. 2(e)]. This is the case also for mode $k = 3800$ [$C_{ee}^{3800}(t)$] but under a higher amount of nonlinearity ($\lambda = 1.0$) and with a slightly lower decaying exponent of $\mu \simeq 0.66$ [see Fig. 2(c)]. In fact, for $\lambda = 1.0$ all the three Anderson modes already decay in a power law [see Fig. 2(f)]. The distinction is that both $C_{ee}^{200}(t)$ and $C_{ee}^{2000}(t)$ decay as $t^{-0.11}$ with a quite long-time tail.

The above tendency can be identified more readily from Figs. 2(a)–2(c). Indeed, in Fig. 2(a) (mode $k = 200$) one can already capture the three distinct processes, i.e., the exponential time decay (process 1) and the power-law time decays with a large (process 2) and small (process 3) μ, although in the cases of $k = 2000$ and $k = 3800$, only two processes are shown [see Figs. 2(b) and 2(c)]. The absence of process 2 for mode $k = 2000$ might be induced by its relatively large localization length. One might also infer that to see process 2 for mode $k = 3800$, a larger amount of nonlinearity would be required. However, whatever these rich details are, the appearance of processes 2 and 3 surely indicates new localized mechanisms, distinct from the delocalization of Anderson modes under a small amount of nonlinearity.

5. Application: nonlinearity-dependent thermal conductivity

Bearing the above dynamical details of single Anderson mode's relaxation in mind, we now show how this interesting transition, i.e., the change from the delocalization for a small amount of nonlinearity to a new localization for a strong nonlinearity can be related to the system's λ-dependent thermal conductivity κ. As mentioned, κ can be measured by the usual direct nonequilibrium molecular dynamic simulations as in Refs. [21,27]. In this approach, two ends of the system are first connected to two heat baths with two different temperatures (we mainly use Noose–Hoover thermal bath here, but we have verified that adopting Langevin heat bath leads to almost the same results; we set the baths' temperatures $T_+ = 2$ and $T_- = 1$, respectively, which ensures that the system's averaged temperature is $T = 1.5$ after applying the heat baths for a long time). Adding the heat baths will drive the system to a nonequilibrium steady state and one might find a well-behaved temperature profile that induces the heat current flowing across the system. Finally, the thermal conductivity is measured by $\kappa = JN/(T_+ - T_-)$ according to the Fourier law.

Another method to obtain κ is based on the Green–Kubo formula[28,29]

$$\kappa = \lim_{\tau\to\infty}\lim_{N\to\infty}\frac{1}{k_{\rm B}T^2N}\int_0^{\tau} C_{JJ}(t)\,{\rm d}t, \tag{4}$$

where $C_{JJ}(t) = \langle J(0)J(t)\rangle$ is the total heat current time autocorrelation with $J = \sum_i \dot{x}_i \partial V(x_{i+1} - x_i)/\partial x_i$ the relevant total current.[27] Distinct from the above nonequilibrium approach, here the heat baths (Noose–Hoover or Langevin) are instead added with the same temperature $T = 1.5$ for a long time to derive an equilibrium steady state and then the baths are removed and $\langle J(0)J(t)\rangle$ is computed by the usual ensemble average as that was performed for $C_{ee}^{k}(t)$.

Fortunately, we find that both nonequilibrium and equilibrium methods give quantitatively the same results in the considered disordered model. As some details, figure 3(a) presents some representative results of $C_{JJ}(t)$ for $\lambda = 0.03$, 0.1, and 1. With this, κ is obtained from the Green–Kubo integration (4) [see Fig. 3(b)]. We will not show the relevant details of the nonequilibrium method but give final results of κ versus λ from both approaches in Fig. 3(c). As can be seen, overall a nonmonotonous dependence of κ on λ can be clearly identified, i.e., as λ increases, κ first increases, and reaches its maximum at $\lambda = 0.1$, and finally decreases. In addition to the saturation of κ at $\lambda = 0.1$, two scaling manners of $\kappa \sim \lambda^{1.03}$ for a small λ and $\kappa \sim \lambda^{-0.89}$ for a large λ can be well numerically inferred. This might be attributed to processes 1 and 3, respectively, as shown in the microscopic Anderson mode's relaxation. Such nonmonotonous variation of κ on λ can thus be understood by the transition of delocalization to the new localization demonstrated above at least qualitatively.

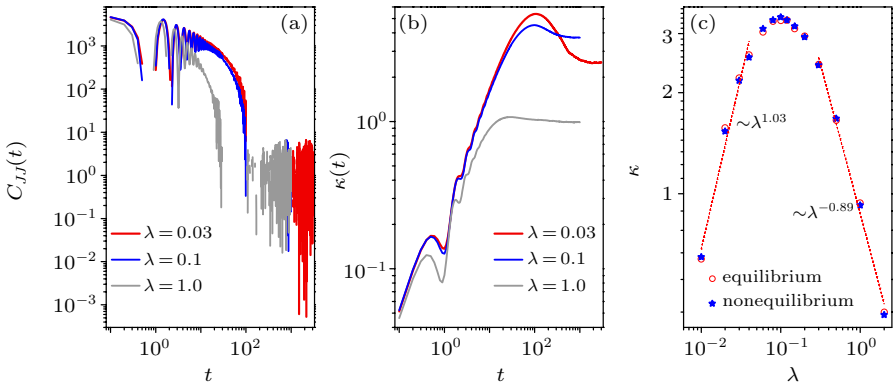


Fig. 3. (a) The total heat current time autocorrelation $C_{JJ}(t)$ for different λ. (b) The measured thermal conductivity κ by equilibrium molecular dynamic (MD) simulations from Green–Kubo formula. (c) κ versus λ, where the data are from both equilibrium and nonequilibrium MD simulations, represented by open and solid symbols, respectively.

6. Discussion and conclusion

To summarize, we have shown that the disorder together with nonlinearity can result in quite rich energy relaxation details of the Anderson modes in the lattice ϕ^4 system. Through studying the time decay of each Anderson mode's energy-energy autocorrelation $C_{ee}^k(t)$, we have revealed that there are generally three relaxation processes with the increase of nonlinearity: (i) process 1: a fast exponential decay, dependent on each mode's localization length; (ii) process 2: a rapid power-law decay, and (ii) process 3: a slow power-law decay. Both processes 2 and 3 are irrelevant to each Anderson mode's localization length, since compared to the rapid delocalization suggested by process 1 they point to new localization mechanisms. These results add new knowledge to further understanding the role of nonlinearity (temperature) played in 1D disordered systems, as such a transition from delocalization to localization has been verified to be relevant to the nonmonotonous variation of thermal conductivity with nonlinearity. They could also be related to the temperature dependence of thermal conductivity in similar models, as the effects of changing temperature could be equivalently explored by changing nonlinearity. As an illustrating example, we note that a work[30] has captured two temperature dependent scaling manners of thermal conductivity with positive exponents for the asymptotic low temperature and intermediate temperature, respectively, which seem to be strongly related to our observed processes 1 and 2. Finally, we would like to point out that we have only considered the effects of hard-type nonlinearity on relaxation here, our study thus also raises one open question: Could the soft-type[31] nonlinearity together with disorder lead to different situations, and are these related to the property of discrete breathers,[32,33] a particular type of spatially localized nonlinear vibrational modes in defect-free nonlinear lattices?

References

[1] Shepelyansky D L 1993 *Phys. Rev. Lett.* **70** 1787
[2] Pikovsky A S and Shepelyansky D L 2008 *Phys. Rev. Lett.* **100** 094101
[3] Chen S D, Zhang Y, Wang J and Zhao H 2013 *Sci. China-Phys. Mech. Astron.* **56** 1466
[4] Kopidakis G, Komineas S, Flach S and Aubry S 2008 *Phys. Rev. Lett.* **100** 084103
[5] Hou Q W and Cao B Y 2012 *Chin. Phys. B* **21** 014401
[6] Flach S, Krimer D O and Skokos C 2009 *Phys. Rev. Lett.* **102** 024101
[7] Xu R F, Han K and Li H P 2018 *Chin. Phys. B* **27** 026801
[8] Skokos C, Gkolias I and Flach S 2013 *Phys. Rev. Lett.* **111** 064101
[9] Guo P, Pan Y K, Li L L and Tang B 2017 *Chin. Phys. B* **26** 073101
[10] Senyange B, Many Manda B and Skokos C 2018 *Phys. Rev. E* **98** 052229
[11] Zhang Z J, Tang C M, Kang J and Tong P Q 2017 *Chin. Phys. B* **26** 100505
[12] Qi K, Tang M, Cui A X and Fu Y 2012 *Chin. Phys. Lett.* **29** 050505
[13] Schwartz T, Bartal G, Fishman S and Segev M 2007 *Nature* **446** 52
[14] Zhan H F and Gu Y T 2018 *Chin. Phys. B* **27** 038103
[15] Roati G, D'Errico C, Fallani L, Fattori M, Fort C, Zaccanti M, Modugno G, Modugno M and Inguscio M 2008 *Nature* **453** 895
[16] Lahini Y, Avidan A, Pozzi F, Sorel M, Morandotti R, Christodoulides D N and Silberberg Y 2008 *Phys. Rev. Lett.* **100** 013906
[17] Zhou K K, Xu N and Xie G F 2018 *Chin. Phys. B* **27** 026501
[18] Lucioni E, Deissler B, Tanzi L, Roati G, Zaccanti M, Modugno M, Larcher M, Dalfovo F, Inguscio M and Modugno G 2011 *Phys. Rev. Lett.* **106** 230403
[19] Anderson P W 1958 *Phys. Rev.* **109** 1492
[20] Li B, Zhao H and Hu B 2001 *Phys. Rev. Lett.* **86** 63
[21] Dhar A and Lebowitz J L 2008 *Phys. Rev. Lett.* **100** 134301
[22] Wang J, Zhang Y and Zhao H 2016 *Phys. Rev. E* **93** 032144
[23] Matsuda H and Ishii K 1970 *Prog. Theor. Phys. Suppl.* **45** 56
[24] Sales M O, Albuquerue S S and de Moura F A B F 2012 *J. Phys.: Condens. Matter* **24** 495401
[25] Thouless D J 1973 *J. Phys. C* **6** L49
[26] Wang J, He D, Zhang Y, Wang J and Zhao H 2015 *Phys. Rev. E* **92** 032138
[27] Lepri S, Livi R and Politi A 2003 *Phys. Rep.* **377** 1
[28] Green M S 1954 *J. Chem. Phys.* **22** 398
[29] Kubo R, Yokota M and Nakajima S 1957 *J. Phys. Soc. Jpn.* **12** 1203
[30] Flach S, Ivanchenko M and Li N 2011 *Pramana-J. Phys.* **77** 1007
[31] Xiong D 2017 *Phys. Rev. E* **95** 042127
[32] Xiong D, Saadatmand D and Dmitriev S V 2017 *Phys. Rev. E* **96** 042109
[33] Kopidakis G and Aubry S 2000 *Phys. Rev. Lett.* **84** 3236