Spatial shift of lattice soliton scattering in the Fermi-Pasta-Ulam model

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Spatial shift produced in scattering process of lattice soliton is studied in the Fermi-Pasta-Ulam model with anharmonic-limit potential. Kink-shaped and antikink-shaped lattice solitons are excited by kicking one single particle. Different behaviors are discovered in two types of head-on collision: kink-kink-shaped collision and kink-antikink-shaped collision. In both cases, the spatial shift not only depends on the scattering pair of lattice solitons but also depends on their collision configuration, i.e., their phase difference. To make a comparison between integrable and nonintegrable lattices, and also to check our method, the Toda model is revisited.

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About half a century ago, Fermi *et al.* discovered the famous paradox of Fermi-Pasta-Ulam "(FPU) recurrence" [1], relating directly to the fundamental, physical, and mathematical problem of energy equipartition and ergodicity in nonlinear systems, which led to the birth of soliton science [2]. By reducing the FPU model to Korteweg–de Vries (KdV) equation in continuum limit, Zabusky and Kruskal numerically observed the named "soliton" [3]. Besides the remarkable stability of soliton, they also noticed that the space-time trajectory of soliton deviates from straight line when one passes through another one. This is a Brief Report about the spatial shift of soliton. Subsequent studies rigorously confirmed these observations and clarified that the spatial shift is essentially connected with the phase shift of soliton that occurred in the scattering process [4]. Making no distinction, it is usually called phase shift in the following studies [5]. The spatial (or phase) shift is an intrinsic property of soliton, which contains the asymptotic information on the effect of soliton interaction and thus is an interesting entity in itself.

So far, almost all of the studies about the spatial shift of soliton focus on those appearing in continuous nonlinear systems which are integrable or nearly integrable [6]. In these systems, solitons may interact without exchanging energy and momentum simply by producing phase shifts. For this situation, soliton interaction can be well described by the phase shift. More than that, such an interaction limits the accessible phase space of system [7], and thus the phase shift can be used to determine correct counting of system state, which provides a basis for a full configurational approach to the statistic mechanics [8].

Recently, solitary waves appearing in discrete nonlinear systems, especially in nonlinear periodic lattices, have been attracting increasing research attention [9]. To contrast their properties with solitons in the continuous systems, they are often referred to as "lattice soliton," "L-soliton" for short in this Brief Report. On the one hand, experimental evidences reveal that L-soliton may present in a variety of systems, e.g., solids [10], biological molecules [11], optical materials [12], etc., where discreteness plays an important role and thus the continuous approximation is not appropriate. For insight into the dynamical and thermodynamical properties of these systems requires knowledge of the detailed information of L-solitons. On the other hand, as one type of dynamical energy localization, L-soliton shows a close connection with the anomalous energy transport phenomena [13]. In fact, such dynamical driven localized modes provide a new window into the underlying simplicity of nonequilibrium processes and thus are of importance in establishing the connections between dynamical behaviors and statistical properties [9].

L-soliton can be excited in perfect nonlinear lattices, as a result of the interplay between discreteness and nonlinearity, which has been predicted for about two decades in theory [14]. In practice, L-soliton is first reported in a special exponential lattice, i.e., the famous Toda model, which is integrable and has the kink-shaped solution [15]. Detailed studies reveal that such a solution behaves the same as that obtained in continuous system, including its spatial shift [4]. For generic nonlinear lattices, however, it was not until recently that L-solitons are worked out [16]. Although the exact solutions of such L-solitons are still lacking, long-lived ones appear in various numerical studies [17]. Such a long-lived L-soliton behaves quite different from its counterparts obtained in the integral systems: energy transfer carries out when they interact with each other; phase difference sensitively affects the scattering process. These nonsolitonlike behaviors, generally attributed to the effect of discreteness, are significant in understanding those fundamental hypotheses of statistical mechanics, e.g., the equipartition of energy and ergodicity of phase space, and thus are desired to be studied quantitatively. Just recently, conservation laws of momentum and energy have been established for the scattering of L-solitons [17]. Unfortunately, as a dominant factor in the interaction of L-solitons, the phase shift still lack quantitative study.

In this Brief Report, we quantitatively study the spatial shift of L-solitons which is the resulting signature of phase shift that occurred in their scattering process. FPU lattice with anharmonic-limit potential is employed as the paradigmatic model since it has been proven to be more suitable for studying the behavior of L-soliton [17]. Because exact solutions of L-soliton still have not been found, numerical method will be applied.

To show the reliability of numerical method, we begin with computing the spatial shift of soliton in Toda model

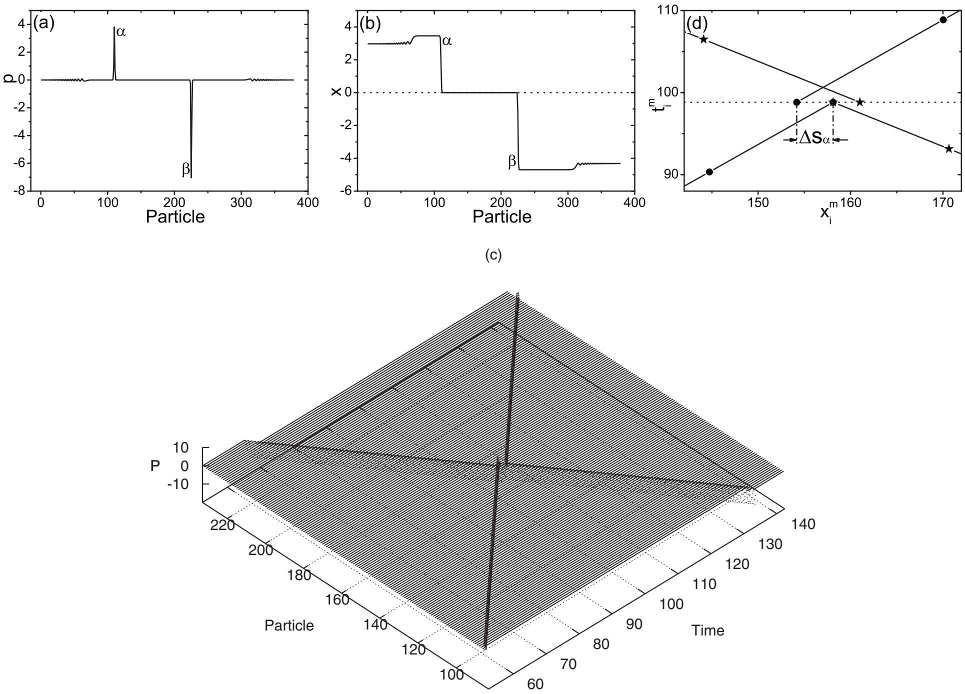

FIG. 1. A pair of solitons excited by $p_1=5$ and $p_N=-10$ in Toda model: (a) the snapshot of particle momentum; (b) the snapshot of particle displacement; (c) the scattering process; the (d) the space-time trajectories.

which is described by $H=\Sigma_{i=1}^{N}[\frac{p_i^2}{2}+V(x_{i+1}-x_i)]$ with $V(x)=e^{-x}+x-1$ [15]. Here, x_i is the displacement of ith particle and p_i is the momentum. It is known that such a system has kink-shaped solutions, $x_n=\ln\frac{1+e^{-(\kappa n-\omega t)}\cdot e^{\kappa}}{1+e^{-(\kappa n-\omega t)}}$, with velocity $v=\frac{2\omega}{\kappa}$ [4], where $\omega=\pm\sinh(\frac{\kappa}{2})$ and the κ determines the extremum of the displacement of particle, denoted by h, when a soliton passes through.

In our numerical studies, the Toda model is initialized as $p_i=0$ and $x_i=0$ for $i=1,\ldots,N$. The soliton is then excited by kicking one single particle, e.g., $p_i=c$ [17,18]. To study soliton scattering, we apply one kick $p_i=c_1$ at $t=0$ and the other $p_j=c_2$ at $t=\delta$ under free boundary condition. Particles i and j should be chosen properly to make sure expected collisions take place. As an example, we consider a system with $N=378$ and take $p_1=5$ and $p_N=-10$ at $t=0$. Figures 1(a) and 1(b) show the snapshots of system at $t\approx 70$. One may notice that there are two supersonic localized excitations, i.e., solitons, denoted by α and β, and each of them is accompanied by a subsonic "tail." These are agreed with previous reports [15]. The soliton velocity is obtained by $v=\frac{x_i^m-x_j^m}{t_i^m-t_j^m}(i\neq j)$, where x_i^m is the position of ith particle at which p_i reaches its extremum and t_i^m is the corresponding time. Parameter h (or κ) is measured directly.

Figure 1(c) shows the collision process of the solitons excited above. To get a better view, the tails have already been wiped off by setting $p_i=0$ and $x_i=h_{\alpha(\beta)}$, where $h_{\alpha(\beta)}$ is the maximal displacement of ith particle induced by soliton $\alpha(\beta)$. Recording x_i^m and t_i^m, one can get their space-time trajectories. As is already known, the soliton preserves its shape and velocity before and after collision and only suffers some spatial shift; thus, the corresponding trajectories are parallel, as shown in Figs. 1(c) and 1(d). The spatial shift of soliton α, denoted by ΔS_α, is marked on Fig. 1(d), which can be measured by extrapolating the space-time trajectories of soliton.

The spatial shift directly measured from the space-time trajectory (e.g., ΔS_α) should be separated into two parts

$$\Delta S_\alpha=\Delta_\alpha\pm h_\beta, \tag{1}$$

where positive sign is taken for $v_\alpha v_\beta>0$ and $|v_\alpha|>|v_\beta|$, i.e., soliton α is the faster one in the overtaking collision; otherwise, minus sign is taken. The reason is as follows. For kink-shaped solitons, ith particle has two equilibrium positions, i.e., $x_i=0$ and $x_i=h$ [12]. Before collision, ith particle has already switched from $x_i=0$ to $x_i=h_\beta$ because soliton β passed. This fact leads the position of soliton α to additionally shift h_β after it interacts with the soliton β. Since h_β only reflects the property of soliton β, it is reasonable to remove it from ΔS_α to get information of soliton interaction. The Δ_α reveals the relative phase shift of soliton α [4,8]. Here, we should mention that Δ_α is independent of time delay δ in Toda model.

Figure 2 shows the results of Δ_α for different h_α. Here, we fix soliton β as $|h_\beta|\approx 3.46$ corresponding to $|c|=5$ and

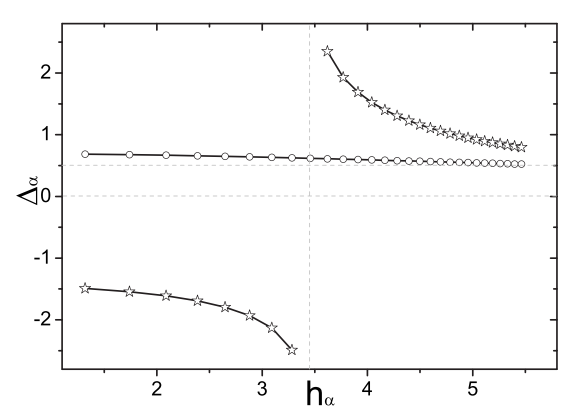

FIG. 2. Δ_α with different h_α obtained by numerical method (stars for head-on collision, circles for overtaking collision) and exact two-soliton solutions (solid line), fixing $|h_\beta|\approx 3.46$.

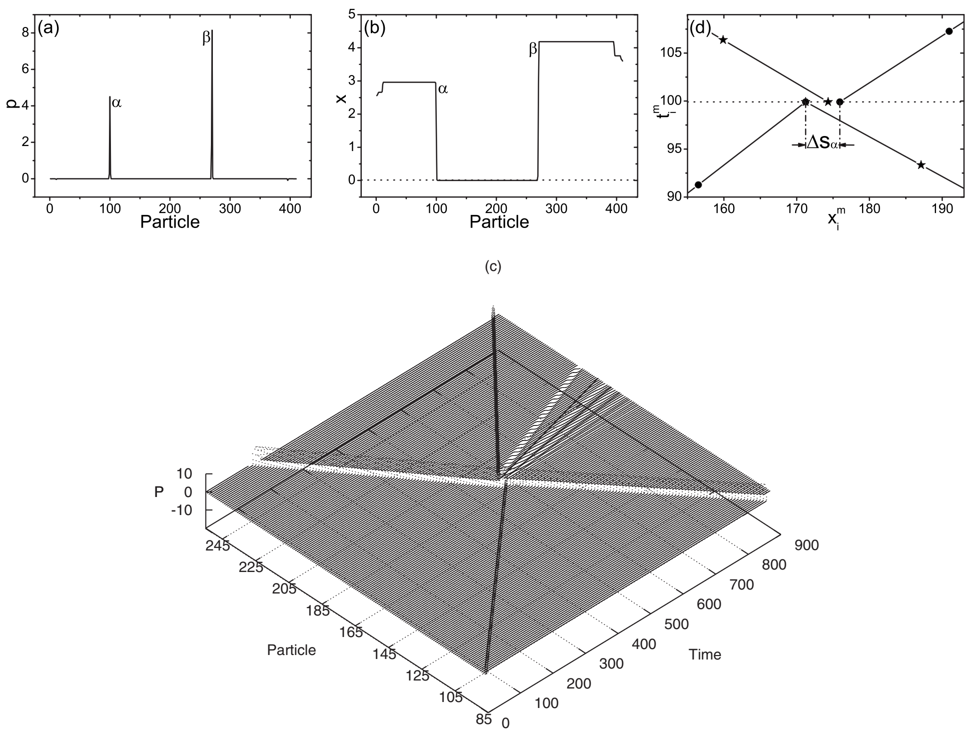

FIG. 3. A pair of L-solitons excited by $p_1=5$ and $p_N=10$ in FPU model: (a) the snapshot of particle momentum; (b) the snapshot of particle displacement; (c) the scattering process; and (d) the space-time trajectories.

change soliton α with $h_\alpha>0$: overtaking collision is considered for $h_\beta>0$; head-on collision is considered for $h_\beta<0$. For comparison, results obtained by the numerical method mentioned above and by the exact two-soliton solutions reported in Ref. [4] have been shown. Clearly, they are perfectly matched with each other. Up to now, we have shown how numerical method is applied to measure the spatial shift of soliton and have checked its reliability. We then apply it to study the spatial shift of L-solitons scattering in FPU model.

The anharmonic-limit version of FPU model, described as $H=\Sigma_{i=1}^{N}[\frac{p_i^2}{2}+\frac{1}{4}(x_{i+1}-x_i)^4]$, is adopted, which shows great superiority to study the dynamics of L-solitons [17]. This system has two types of L-soliton solutions [16]: one is kink-shaped solution moving in the same direction as that of the particle; another is antikink-shaped solution whose moving direction is opposite to that of the particle. Examples are shown in Figs. 3(a) and 3(b), obtained in the system with $N=410$ by taking kicks $p_1=5$ and $p_N=10$ at $t=0$, respectively, denoted as α and β. Here, the α is a kink-shaped L-soliton and β is a antikink-shaped one. Both are accompanied by smaller L-solitons that will be wiped off to get a better view of the collision process as it does in the Toda model.

Figure 3(c) shows the collision process of the L-solitons produced above. One can notice that some new waves are excited during the collision. This means that the total energy of above L-solitons is reduced but not necessarily implies every one of them loses its energy. Previous studies reveal that the smaller L-soliton gains energy in the scattering process, while the bigger one loses energy [17]. Since the energy is changed, the speed of L-soliton will be different before and after the collision, and thus the corresponding space-time trajectories are no longer parallel as shown in Figs. 3(c) and 3(d). Of course, collision also produces spatial shifts. As an example, spatial shift of L-soliton α, ΔS_α, is marked on Fig. 3(d), which can be directly measured by extrapolating the space-time trajectories.

This Brief Report focuses on studying the spatial shift produced from two types of head-on collisions: (1) collision between the same types of L-solitons; (2) collision between different types of L-solitons. Again, the directly measured spatial shift (e.g., ΔS_α) should be separated by (1) to obtain the information of L-soliton interaction as it is mentioned in the case of Toda model. Minus sign will be taken.

First, motivated by previous reports [17], we study the relationship between Δ_α and δ. Some typical results are shown in Fig. 4(a), which reveal them to be clearly periodic. In fact, such behavior originates in the discrete nature of lattice. For a certain pair of L-soliton, different δ is equivalent to different collision configuration because head-on collision is essentially an exchange effect. Let us suppose that particles i_α and i_β belong to L-soliton α and β, respectively. During the scattering process, there must be a time t_c when particle i_α and i_β reach the same velocity v_c. Here, $i_\beta=i_\alpha\pm1$ or ±2. When $t>t_c$, particle i_α will belong to L-soliton β and i_β will belong to α; the exchange (or collision) is finished. It is easy to find the following special configurations: (a) $i_\beta=i_\alpha\pm2$ and $v_c=0$, ΔS_α reaches the maximal value; (b) $i_\beta=i_\alpha\pm1$ and $v_c=min\{v_{i_\alpha}^m,v_{i_\beta}^m\}$, ΔS_α reaches the minimal value; and (c) $i_\beta=i_\alpha\pm1$ and $v_c=0$, ΔS_α reaches the intermediate value. Here, $v_{i_\alpha}^m$ and $v_{i_\beta}^m$ are the maximal velocity that particle i_α and i_β can reach. The periodicity reflects the period of lattice model.

Then, we study how the spatial shift depends on the scattering pair of L-solitons. For this purpose, the mean value $\langle\Delta_\alpha\rangle$ is of more significance than the prompt value. Without loss of generality, we change the L-soliton α with $h_\alpha>0$ and fix β as $|h_\beta|\approx2.96$ corresponding to $|c|=5$: kink-kink-shaped

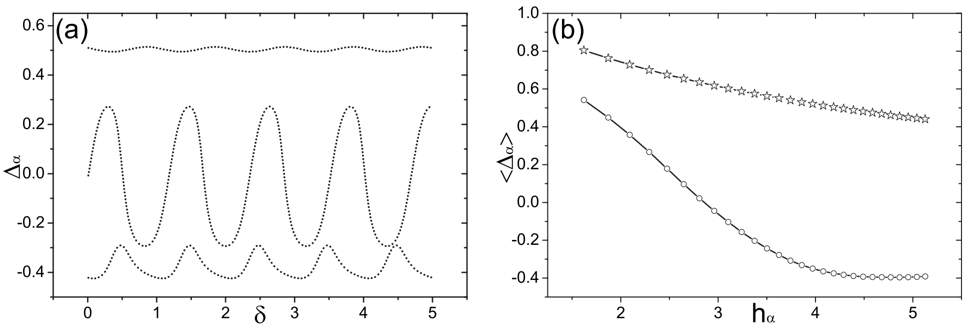

FIG. 4. (a) Δ_α vs δ (from top to bottom: $h_\alpha \approx 4.19$ and $h_\beta \approx -2.96$, $h_\alpha \approx 2.96$ and $h_\beta \approx -2.96$, $h_\alpha \approx 4.19$ and $h_\beta \approx 2.96$); (b) $\langle\Delta_\alpha\rangle$ vs h_α (stars for kink-kink-shaped head-on collision with $h_\beta \approx -2.96$, circles for kink-antikink-shaped head-on collision with $h_\beta \approx 2.96$).

collision takes place when $h_\beta < 0$; kink-antikink-shaped collision happens when $h_\beta > 0$. Results are shown in Fig. 4(b). Each $\langle\Delta_\alpha\rangle$ is gained by averaging over several periods of Δ_α. Clearly, $\langle\Delta_\alpha\rangle$ decreases with the increase in h_α for both types of collision. Meanwhile, the difference is also apparent: there always is $\langle\Delta_\alpha\rangle > 0$ for kink-kink-shaped collision; while $\langle\Delta_\alpha\rangle > 0$ for $h_\alpha < h_\beta$ and $\langle\Delta_\alpha\rangle < 0$ for $h_\alpha > h_\beta$ in the case of kink-antikink-shaped collision. These behaviors have not been observed in the continuum approximation [4].

Finally, we emphasize here that Δ_α cannot be directly regarded as the relative phase shift of soliton α because L-soliton α is intrinsically changed to another one $\tilde{\alpha}$ after the collision. To obtain the information of phase change, based on *prior* knowledge [16,19], we suppose the kink-shaped solution of FPU model satisfies $u(x,t) = \Phi(\kappa x \pm \omega t)$. Here, ω is inverse of the period that a particle reaches its maximal displacement starting from when it began to move. Numerical studies suggest that $\omega = c_1 h + c_2$, where $c_1 \approx 0.085\,37$ and $c_2 \approx 0.002\,56$. Considering the previous result $v = \frac{\omega}{\kappa} = \frac{h}{\sqrt{3}}$ [17,18], one can get $\kappa = \frac{\sqrt{3}}{h}(c_1 h + c_2)$. Then, the phase difference between L-soliton α and $\tilde{\alpha}$ can be written as $\Delta\phi_\alpha = \sqrt{3}c_1(x_{\tilde{\alpha}} - x_\alpha) + \sqrt{3}c_2(\frac{x_{\tilde{\alpha}}}{h_{\tilde{\alpha}}} - \frac{x_\alpha}{h_\alpha})$, setting the collision time $t_c = 0$. Since the second term of right-hand side is negligibly small compared to the first one, above equation can be reduced to

$$\Delta\phi_\alpha \approx \sqrt{3}c_1(x_{\tilde{\alpha}} - x_\alpha) = \sqrt{3}c_1 \Delta S_\alpha. \tag{2}$$

Therefore, Δ_α approximately reveals the phase change of L-soliton α caused by the collision.

In summary, we have studied spatial shifts of L-soliton in the FPU model with anharmonic-limit potential. It is found that the spatial shift not only depends on the collision pair of L-solitons but also depends on their collision configuration, i.e., their phase difference. For a given pair of L-solitons, the spatial shift periodically changes with the delay time δ. More importantly, it is discovered that the behavior of spatial shift obtained in kink-kink-shaped collision is very different from that obtained in kink-antikink-shaped collision. These properties are essentially different from that of the solitons satisfying the KdV equation which is one continuous approximation of FPU model.

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[1] E. Fermi *et al.*, Los Alamos Scientific Laboratory Report No. LA-1940, 1955 (unpublished).
[2] M. Remoissenet, *Waves Called Solitons* (Springer-Verlag, Berlin, 1999).
[3] N. J. Zabusky and M. D. Kruskal, Phys. Rev. Lett. **15**, 240 (1965).
[4] P. D. Lax, Commun. Pure Appl. Math. **21**, 467 (1968); M. Wadati and M. Toda, J. Phys. Soc. Jpn. **32**, 1403 (1972); **34**, 18 (1973).
[5] H. Ikezi *et al.*, Phys. Rev. Lett. **25**, 11 (1970); R. Hirota and K. Suzuki, Proc. IEEE **61**, 1483 (1973); K. Nakajima *et al.*, Phys. Rev. Lett. **65**, 1667 (1990); M. Wu and C. E. Patton, *ibid.* **98**, 047202(2007).
[6] Y. S. Kivshar and B. A. Malomed, Rev. Mod. Phys. **61**, 763 (1989).
[7] J. F. Currie *et al.*, Phys. Rev. B **22**, 477 (1980); N. Theodorakopoulos, Z Phys. B **46**, 367 (1982); Phys. Rev. B **30**, 4071 (1984).
[8] J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B **11**, 3535 (1975); N. Theodorakopoulos and F. G. Mertens, *ibid.* **28**, 3512 (1983); N. Theodorakopoulos, Phys. Rev. Lett. **53**, 871 (1984); N. Theodorakopoulos and M. Peyrard, *ibid.* **83**, 2293 (1999).
[9] S. Flach and C. R. Willis, Phys. Rep. **295**, 181 (1998); M. Sato *et al.*, Rev. Mod. Phys. **78**, 137 (2006).
[10] U. T. Schwarz *et al.*, Phys. Rev. Lett. **83**, 223 (1999).
[11] A. Xie *et al.*, Phys. Rev. Lett. **84**, 5435 (2000).
[12] J. W. Fleischer *et al.*, Nature (London) **422**, 147 (2003).
[13] B. Hu *et al.*, Phys. Rev. E **61**, 3828 (2000); Hong Zhao, Phys. Rev. Lett. **96**, 140602 (2006).
[14] A. S. Dolgov, Sov. Phys. Solid State **28**, 907 (1986); A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[15] M. Toda, *Theory of Nonlinear Lattices* (Springer-Verlag, Berlin, 1981).
[16] J. Szeftel *et al.*, Phys. Rev. Lett. **83**, 3982 (1999).
[17] H. Zhao *et al.*, Phys. Rev. Lett. **94**, 025507 (2005); R. Khomeriki, Phys. Rev. E **65**, 026605 (2002); S. V. Dmitriev, *et al.*, *ibid.* **66**, 046609 (2002); Yu. Doi, *ibid.* **68**, 066608 (2003); E. McMillan, Physica D **200**, 25 (2005).
[18] R. Dusi *et al.*, Phys. Rev. B **54**, 9809 (1996).
[19] G. Friesecke and J. A. D. Wattis, Commun. Math. Phys. **161**, 391 (1994).