

Influence of the bond defect in driven Frenkel-Kontorova chains

Huan Xu, Weizhong Chen,* and Yifei Zhu

Key Laboratory of Modern Acoustics and Institute of Acoustics, Nanjing University, Nanjing, 210093, China

(Received 6 April 2007; published 11 June 2007)

We study the influence of a bond defect in a nonlinear coupled pendulum chain subjected to vertical vibration experimentally. We observe that the defect can attract or repel solitons including phase-matched breather, phase-mismatched breather, and phase-mismatched kink. Furthermore, we observe a new phenomenon that the interaction polarity is dependent on the location of the defect in the phase-matched breather. If a defect locating near a breather center attracts the breather, it will repel the breather when it locates at a further place. And the effects of the defect on the phase-mismatched solitons are similar to the phenomena observed in the studies on the pendulum length defects. We also find the interaction intensity is related to the defect intensity.

DOI: 10.1103/PhysRevB.75.224303

PACS number(s): 05.45.Xt, 61.72.Bb, 63.20.Pw

I. INTRODUCTION

The Frenkel-Kontorova (FK) model describes the dynamics of a chain of particles interacting with the nearest neighbors in an external periodic potential.¹ The model and its generalizations are widely applied in investigating physical phenomena related to crystal structures, for example, Josephson junctions,² the sliding friction,³ and commensurate-incommensurate phase transitions.⁴ A number of current researches, such as electronic conductance in nanotubes,⁵ quantum-creep transitions,⁶ and heat conduction,^{7,8} are also carried out with the help of the model. In fact, most crystal surfaces contain different types of defects, such as chemisorbed or adsorbed species, vacancies, and interstitial atoms. All of them lead to bond defects in lattice, and people have paid more attention to the influence of defects. They extend the model to the case with some defects and get considerable fruits.^{1,9-13} In 1991, Braun and Kivshar⁹ found that local defects modified transport properties of one-dimensional systems, and the kink diffusion coefficient depended on the character of the kink interaction with a single defect (repulsion or attraction). A recent study¹⁰ pointed out that a chemical bond defect could stimulate the formation of both double-kink and kink-antikink pair. The similar phenomena could be found in defect-breather interactions: breathers can be trapped, transmitted, or reflected by vacancies.^{11,12} On the other hand, as a macroscopic expression of the FK model, a vertically driven chain of pendulums coupled to their nearest neighbors is widely investigated both in numerical simulations^{14,15} and experiments.¹⁶⁻¹⁹ In the early 1990s, people observed localized kink¹⁶ and breather¹⁷ in the chain experimentally. Various defects were also introduced into the uniform chains, and many fabulous phenomena were observed. For example, a single defective pendulum could tame the complex chaotic behavior in a very long chain of pendulums.¹⁵ Additionally, a single defect in an FK chain could also attract or repel solitary waves.^{14,18,19} Although the effects of the bond defects have been catching much attention in crystal physics,^{20,21} in previous work, the defects that have been studied in the pendulum chain are always in pendulum length or mass. Few of the bond (coupling) defects have been studied. Therefore, it is necessary to research a

pendulum chain with coupling defects. In our paper, we experimentally study the coupling defect in this driven FK chain. Following this introduction, the experimental apparatus are presented in Sec. II. Sections III and IV are the experimental investigations on the effect of the coupling defect on the phase-matched solitons and phase-mismatched solitons, respectively. The experimental results are compared with the studies on the pendulum length defects in the two sections. The observations are proved numerically in Sec. V. The dissertation concludes with an overall summary of the research in Sec. VI.

II. PENDULUM CHAIN

As shown in Fig. 1, N steel pendulum balls with the same mass m were suspended on a beam. They were uniformly arranged in a horizontal line with equal spacing a to each other. Each ball was hung by two strings in a shape similar to the letter V and coupled with its nearest neighbors by gathering the strings using a small light tube which was hung on the beam by a thread (see Fig. 1). The coupling intensity was determined by the coupling length b , *viz.*, the distance from beam to the bottom of the tube. The parameters of the chain were expressed as follows: the pendulum mass $m=3.0$ g, the spacing $a=20.0$ mm, the coupling length $b=24.0$ mm, the number of pendulums $N=43$, and the pendulum length l . It was impossible to observe all solitons in one chain,¹⁷ so we used two chains, whose pendulum lengths were different, $l=82.0$ mm (chain 1) and $l=92.0$ mm (chain 2). The deviations in mass m and length l were less than 3.0 mg and

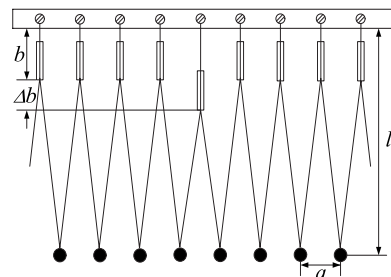


FIG. 1. Pendulum chain.

0.1 mm in our chains, respectively. By changing one thread, we could quickly pull the tube up or down to introduce a coupling defect. If the tube was raised, the coupling became weaker, and vice versa. The defect intensity Δb , the change of b , was limited within 10% of b . Therefore, the introduced coupling defect was small, compared with the coupling length. The pendulum length of two neighbor pendulums could be regarded as constant when the coupling length was slightly changed. The experimental apparatus consisted of three parts: the chains, the vibration part, and the measuring one (see Ref. 18). The chain was fixed on a vibration platform driven by a sinusoidal voltage $A_e \cos 2\pi f_e t$. The measuring apparatus mainly included a video camera that recorded the temporal evolution of the solitons. The details of the vibration apparatus and measuring apparatus were described in Ref. 18.

III. EFFECT ON THE PHASE-MATCHED BREATHER

Before introducing a coupling defect, we applied the frequency f_e and the amplitude A_e to the vibration platform to generate nonpropagating solitons.^{16,17} Three kinds of solitons were studied: phase-matched breather, phase-mismatched breather, and phase-mismatched kink. The term phase-matched or phase-mismatched refers to whether the neighbor pendulums swing towards the same or opposite direction. Then a coupling defect Δb was suddenly brought in, and the defect-soliton interaction was observed. If the coupling was boosted up, it was called positive defect, otherwise negative defect.

When chain 1 was driven by $A_e=1.2$ mm at $f_e=3.500$ Hz, a nonpropagating phase-matched breather was generated at a random location.¹⁷ The position of the breather center was set as $x_0=0$. The tube at $x_d=-1.5a$ was quickly lowered by $\Delta b=2$ mm to introduce a positive coupling defect. Then the breather moved towards the defect [see Fig. 2(a)]. On the contrary, when a negative coupling defect was introduced by quickly raising the tube by $\Delta b=-2$ mm at the same location, the breather moved away [see Fig. 2(b)]. These observations were similar to those observed in the experiments on pendulum length defect.¹⁸ However, it was quite astonishing that the interaction polarity would be opposite when the defect was introduced at a further location ($x_d=-2.5a$). In other words, the interaction inverted just due to changing the position of the defect from $-1.5a$ to $-2.5a$. As shown in Fig. 3, the breather was repelled (attracted) when a positive (negative) defect was set at a further location ($x_d=-2.5a$). We can draw the conclusion that the interaction polarity was related to the relative distance between the breather and the coupling defect. This is a new phenomenon that has never been observed in a pendulum chain with pendulum length defects,^{14,18} or in a continuous system with defects.¹⁹ And it strongly suggests that the interaction is dependent on the wave form of the solitons.

IV. EFFECT ON THE PHASE-MISMATCHED SOLITONS

Similarly, experiments on the interaction between a coupling defect and nonpropagating phase-mismatched solitons

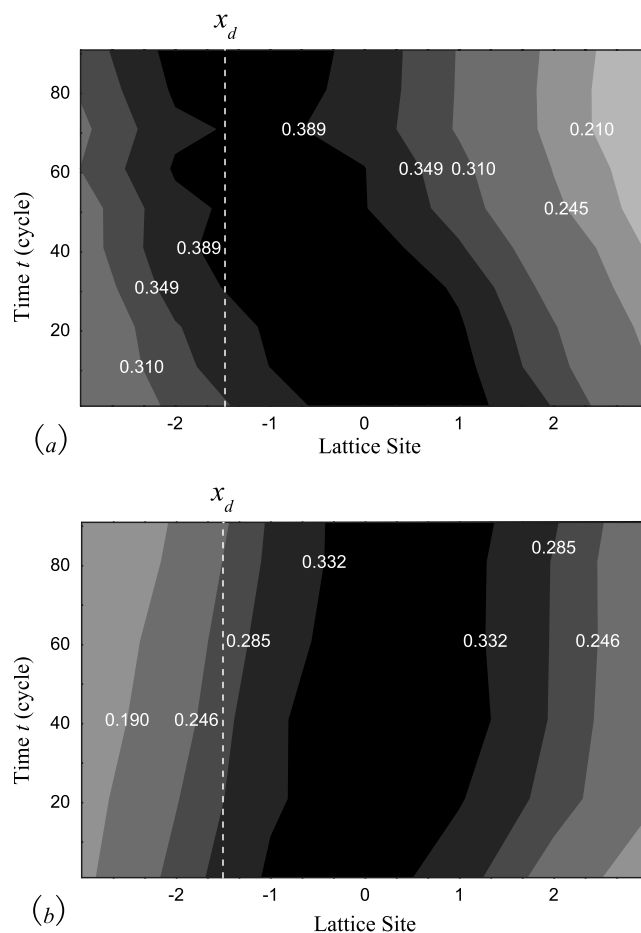


FIG. 2. Effect of a closely located coupling defect on the nonpropagating phase-matched breather. The gray scale values in the maps show the temporal evolution of the pendulum radians. The driving parameters are $A_e=1.2$ mm, $f_e=3.500$ Hz, respectively. (a) A positive defect at $x_d=-1.5a$ attracts a breather ($x_0=0$). (b) A negative one at $x_d=-1.5a$ repels the breather.

were performed in the pendulum chain. Different defect intensities Δb were introduced to study the relationship between the defect intensity and the interaction intensity. To demonstrate the interaction intensity, the experimental data were fitted with exponential decay function $e^{-t/\tau}$, where the characteristic time τ denoted the interaction intensity. The longer τ is, the weaker the interaction is. So the relationship between the defect intensity and the interaction intensity can be described by the relationship between Δb and τ .

A. Positive (negative) defect attracts (repels) the phase-mismatched breather

To observe a phase-mismatched breather, chain 1 was replaced by chain 2. At $A_e=0.75$ mm and $f_e=3.755$, a nonpropagating phase-mismatched breather¹⁷ appeared. A positive coupling defect ($\Delta b=2$ mm) was introduced at $x_d=1.5a$ relating to the breather center $x_0=0$, then the defect attracted the breather and pinned it [see Fig 4(a)]. There was no change of the interaction polarity as we changed the location of the defect. The interaction polarity would change,

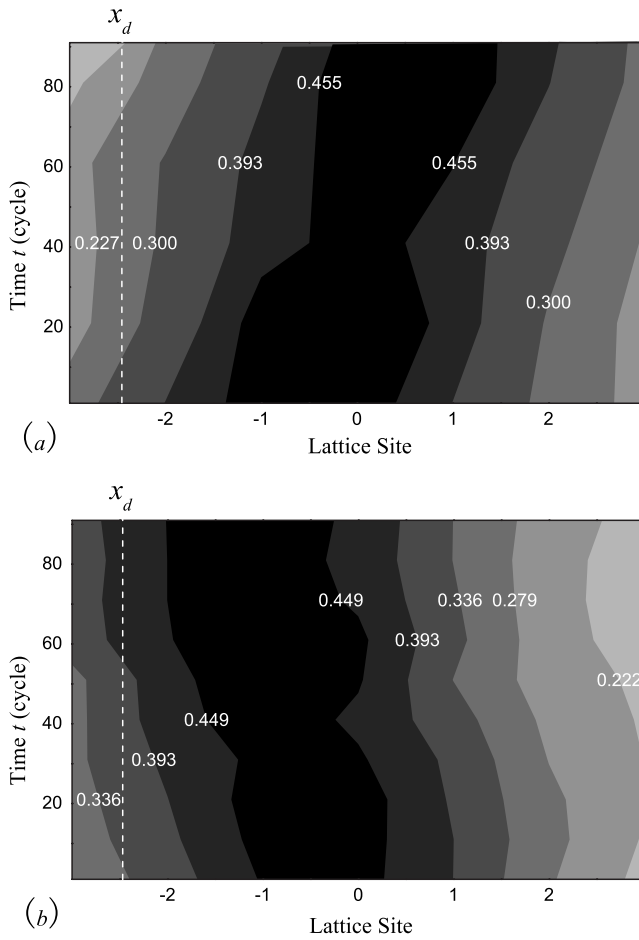


FIG. 3. Effect of a further located coupling defect on the non-propagating phase-matched breather. The gray scale values in the maps show the temporal evolution of the pendulum radii. The driving parameters are $A_e=1.2$ mm, $f_e=3.494$ Hz, respectively. (a) A positive defect at $x_d=-2.5a$ repels a breather ($x_0=0$). (b) A negative one at $x_d=-2.5a$ attracts the breather.

of course, if we introduced a negative defect. Figure 4(b) showed that breathers were repelled by a negative defect $\Delta b=-2$ mm at $x_d=2.5a$. We observed the movements of the solitons after introducing different defect intensities Δb . The experimental results were plotted as mean value of every five cycles together with SD. And the insets of Fig. 4 showed the constant τ at different $|\Delta b|$. In previous literature,¹⁸ the author observed that a long defect repelled phase-mismatched breather, and a short one attracted it. It was obvious that a positive (negative) coupling defect acted the same as a short (long) pendulum length defect. The opposite effect can be interpreted by the energy absorbing theory.¹⁴

B. Positive (negative) defect repels (attracts) the phase-mismatched kink

In order to form a kink, we switched back to chain 1. A nonpropagating phase-mismatched kink¹⁶ generated at $A_e=1.6$ mm and $f_e=4.195$ Hz. We introduced a positive coupling defect ($\Delta b=2$ mm) at $x_d=1.5a$ with respect to the kink center $x_0=0$, then the kink was repelled. On the contrary,

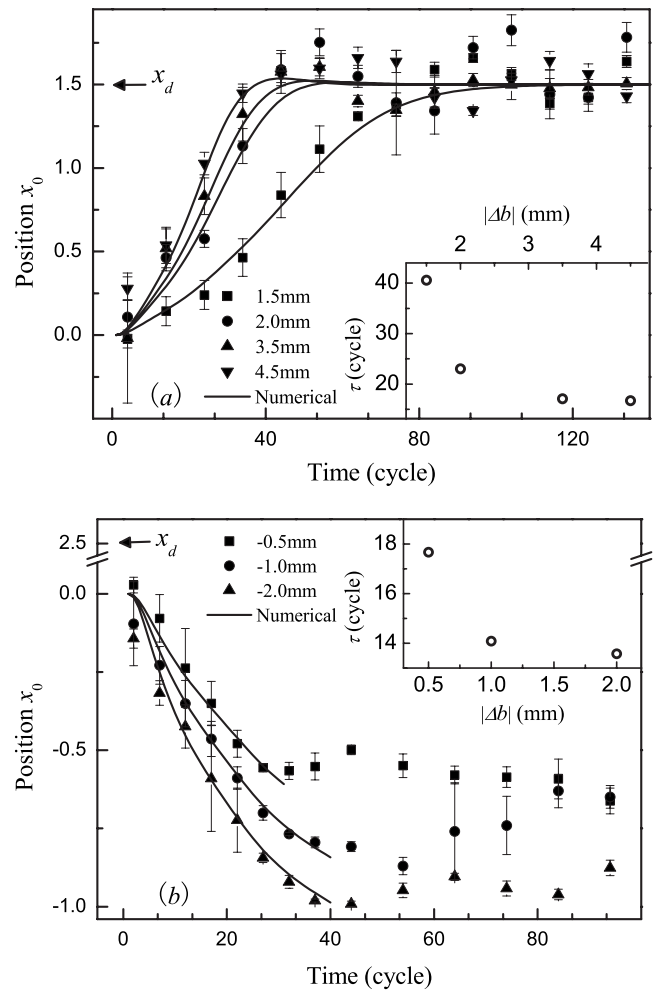


FIG. 4. The interactions between the defect and the phase-mismatched breather. The driving parameters are $A_e=0.75$ mm, $f_e=3.755$ Hz, respectively. (a) A positive defect at $x_d=1.5a$ attracts a breather from $x_0=0$ to x_d , and pins it at x_d . (b) A negative one at $x_d=2.5a$ repels the breather.

after introducing a negative coupling defect ($\Delta b=-2$ mm), the kink moved towards the defect and stopped at it finally. Figure 5 showed the temporal evolution of the kink center, and the insets showed the relationship between Δb and τ . We also observed the opposite effect between a coupling defect and a pendulum length defect¹⁸ under the same condition. The numerical calculations on the bond defect in phase-mismatched kink were done by Braun and Kivshar in 1991.⁹ Considering the change in both the energy of atoms interaction with the substrate and the energy of a pairwise interaction of atoms between themselves, the authors found positive defect potential was repulsive, and a negative one was attractive. Their conclusion was proved experimentally in our experiments.

From the inset pictures of Figs. 4 and 5, it was clear that the characteristic time τ increased with the decreasing of the defect intensity $|\Delta b|$. That is to say that the interaction will be weakened if the defect intensity is decreased, which is also proved in propagating solitons.^{11,12} In the study of Cuevas *et al.*,^{11,12} a vacancy, a kind of negative bond defects, could repel a propagating breather. Furthermore, the propa-

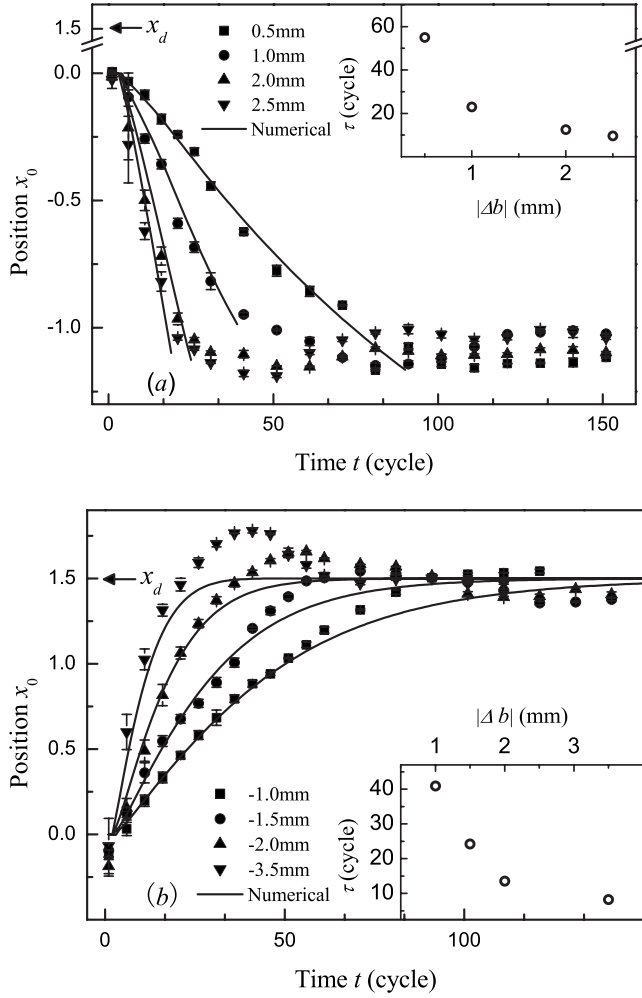


FIG. 5. The interactions between the defect and the phase-mismatched kink. The driving parameters are $A_e = 1.6$ mm, $f_e = 4.195$ Hz, respectively. (a) A positive defect at $x_d = 1.5a$ repels a kink from $x_0 = 0$. (b) A negative one at $x_d = 1.5a$ attracts the kink from $x_0 = 0$ to x_d , and pins it at x_d .

gating breather could go through the vacancy first and then be repelled at a weak defect, however, it would be reflected at a strong one. Comparing Fig. 4 with Fig. 5, a positive coupling defect attracted phase-mismatched breather and repelled phase-mismatched kink, and a negative one played an opposite role. Indeed, the topology of the soliton had an effect on the coupling defect-soliton interactions. The interaction polarity was inverted when the topology of the soliton changed, which agreed with observations in lattice solitons with a pendulum length defect¹⁸ and in hydrodynamic solitons with a width or depth defect.¹⁹

V. NUMERICAL SIMULATION

A. Phase-matched soliton

The radian of the n th pendulum in the chain satisfies the following dynamical equations:

$$\begin{aligned}
 ml^2 \ddot{\theta}_n + \beta l \dot{\theta}_n - k_{2,n,n+1}(\theta_{n+1} - \theta_n) - k_{2,n-1,n}(\theta_{n-1} - \theta_n) \\
 - k_{4,n,n+1}(\theta_{n+1} - \theta_n)^3 - k_{4,n-1,n}(\theta_{n-1} - \theta_n)^3 \\
 = -ml(g + 4\pi^2 A_e f_e^2 \cos 2\pi f_e t) \sin \theta_n \\
 (n = 1, 2, \dots, N).
 \end{aligned} \quad (1)$$

θ_n is the radian of the n th pendulum, $k_{2,n-1,n}$ and $k_{4,n-1,n}$ are the coupling coefficients of harmonic potentials and quartic potentials between the $(n-1)$ th and the n th pendulums. β is the friction coefficient, and g is the acceleration of gravity. Then we take the continuum limit approximation¹⁴ that can keep the basic features of the dynamics of the FK chain. We consider that the coupling defect makes the linear coefficient k_2 change, say $k_2(x)$. Equation (1) can be derived to

$$\begin{aligned}
 \ddot{\theta} + \frac{\beta}{ml} \dot{\theta} - \frac{a^2}{ml^2} [k_2(x) \theta_x]_x - \frac{3a^4}{ml^2} k_4 \theta_x^2 \theta_{xx} \\
 = -\frac{g}{l} \left(1 + \frac{4\pi^2 A_e f_e^2}{g} \cos 2\pi f_e t \right) \sin \theta.
 \end{aligned} \quad (2)$$

Finally, Eq. (2) is expanded to three orders using the multiple scale expansion method,¹⁴ based on the assumptions $\beta = \alpha \varepsilon^2$, $\frac{4\pi^2 A_e f_e^2}{g} = \gamma \varepsilon^2$, $k_2(x) = k_2[1 + qf(x)]$, $f_1 = \frac{1}{2\pi} \sqrt{\frac{g}{l}}$, and $f_e^2 = (2f_1)^2(1 + p\varepsilon^2)$ with ε being a small parameter. f_1 is the intrinsic frequency for phase-matched mode, $f(x)$ is the function describing the coupling defect, and q is the strength of the defect. However, in the equation expanded from Eq. (2), the term with defect is ignored because its order is higher than three orders. Therefore, we use Eq. (1) instead of the expanded equation to investigate the effect of a coupling defect on a phase-matched breather. We plot the trace of the nonpropagating phase-matched breather center after introducing a coupling defect at different locations by resolving Eq. (1) using the fourth-order Runge-Kutta method (see Fig. 6). We can conclude that the relative distance between the coupling defect and the breather affects the interaction polarity, and the numerical calculation results agree with our experimental results. The numerical results also tell us, when the coupling defect is located far away from the breather, the interaction intensity is small.

B. Phase-mismatched soliton

As for phase-mismatched solitons, different from the case of phase-matched solitons, we will get the nonlinear Schrödinger equation with a coupling defect term [Eq. (4)] after doing the same algebra to Eq. (1). In brief, we take the continuum limit approximation¹⁴ to get Eq. (3), then expand Eq. (3) using multiple scale expansion method. Assuming $\varphi_n = (-1)^n \theta_n$, we obtain

$$\begin{aligned}
 \ddot{\varphi} + \frac{\beta}{ml} \dot{\varphi} + \frac{k_2(x)}{ml^2} (4\varphi + a^2 \varphi_{xx}) \\
 + \frac{k_2'(x)}{ml^2} a^2 \varphi_x + 2k_4 \left(2\varphi + \frac{a^2}{2} \varphi_{xx} \right)^3 \\
 = -\frac{g}{l} \left(1 + \frac{4\pi^2 A_e f_e^2}{g} \cos 2\pi f_e t \right) \sin \varphi.
 \end{aligned} \quad (3)$$

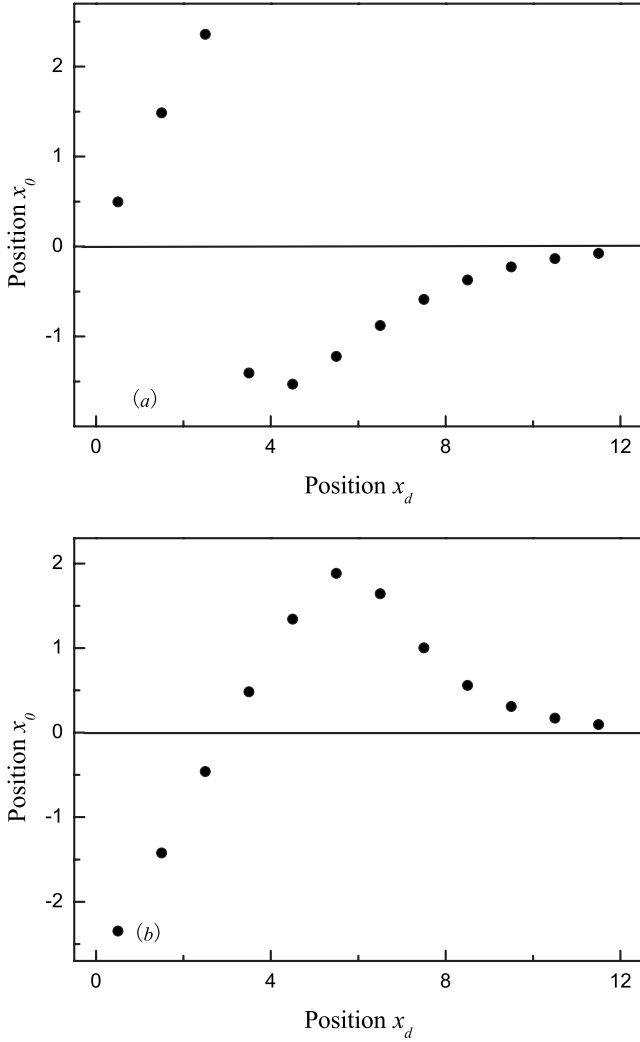


FIG. 6. 300 s after introducing a coupling defect at different locations, the positions of a phase-matched breather center. The defect intensity is $|q|=0.1$ and the initial position of breather center is $x_0=0$. (a) The interaction polarity changes with the position of a positive defect ($q=0.1$). (b) The interaction polarity changes with the position of a negative one ($q=-0.1$).

φ can be written as $\varphi = \phi \exp j2\pi f_2 t + \text{c.c.}$ ϕ satisfies

$$j4\pi f_2 \phi_t + \frac{k_2 a^2}{ml^2} \phi_{xx} + \left(\frac{4k_2}{ml^2} q f(x) - 4\pi^2 f_2^2 p \right) \phi + \frac{j2\pi f_2 \alpha}{ml} \phi + \left(\frac{48k_4}{ml^2} - \frac{g}{2l} \right) |\phi|^2 \phi + \frac{g\gamma}{2l} \phi^* = 0, \quad (4)$$

here $f_2 = \frac{1}{2\pi} \sqrt{\frac{g}{l} + \frac{4k_2}{ml^2}}$, and $f_e^2 = (2f_2)^2 (1 + p\varepsilon^2)$. f_2 is the intrinsic

TABLE I. Experimental results.

Soliton	Defect	Interaction
Matched breather(near)	Positive	Attract
	Negative	Repel
Matched breather(far)	Positive	Repel
	Negative	Attract
Mismatched breather	Positive	Attract
	Negative	Repel
Mismatched kink	Positive	Repel
	Negative	Attract

frequency for phase-mismatched mode. We fit the experimental data by resolving Eq. (4) using fourth-order Runge-Kutta method (see curves in Figs. 4 and 5). Generally, there is good agreement between the experimental and fitting results. But, at the later stage, the experimental data cannot be fitted well. We believe that it relates to the difference between a continuous system and a discrete one. Equation (4) is a continuous model, so the moving of the breather is smooth and the repulsive progress will not stop. However, the pendulum chain is a discrete system and the moving soliton is blocked by potential barrier. Therefore, We can observe the soliton vibrating between two neighbor pendulums, which is called overstepping,¹⁸ in the interaction between the coupling defect and the soliton.

VI. CONCLUSION

Our experimental results show that a coupling defect can attract or repel the solitons including breather and kink. A new phenomenon that has never been referred to in previous literature of the pendulum chain^{14,18} is observed in the experiments on the interaction between the nonpropagating phase-matched breather and a coupling defect: the relative distance between the breather center and the coupling defect has a role in the polarity of the interaction (Table I). And in the experiments on the interaction between the coupling defect and the nonpropagating phase-mismatched solitons (Table I), we observe that both the topology of the soliton and the coupling defect play a role in the characteristic of the interaction. Furthermore, the defect intensity affects the interaction intensity: the interaction will be stronger if the strength of the coupling defect is increased.

ACKNOWLEDGMENT

This work was supported by the National Natural Science Foundation of China (Grant No. 10434070).

*Corresponding author; wzchen@nju.edu.cn

- ¹O. M. Braun and Y. S. Kivshar, *Phys. Rep.* **306**, 1 (1998).
- ²L. M. Floria and J. J. Mazo, *Adv. Phys.* **45**, 505 (1996).
- ³S. Goncalves, C. Fusco, A. R. Bishop, and V. M. Kenkre, *Phys. Rev. B* **72**, 195418 (2005).
- ⁴A. S. Kovalev, I. V. Gerasimchuk, and G. A. Maugin, *Phys. Rev. Lett.* **92**, 244101 (2004).
- ⁵L. S. Levitov and A. M. Tsvelik, *Phys. Rev. Lett.* **90**, 016401 (2003).
- ⁶F. R. Krajewski and M. H. Muser, *Phys. Rev. Lett.* **92**, 030601 (2004).
- ⁷A. V. Savin and O. V. Gendelman, *Phys. Rev. E* **67**, 041205 (2003).
- ⁸B. W. Li, L. Wang, and G. Casati, *Appl. Phys. Lett.* **88**, 143501 (2006).
- ⁹O. M. Braun and Y. S. Kivshar, *Phys. Rev. B* **43**, 1060 (1991).
- ¹⁰Y. N. Gornostyrev, M. I. Katsnelson, A. Y. Stroev, and A. V. Trefilov, *Phys. Rev. B* **71**, 094105 (2005).
- ¹¹J. Cuevas, C. Katerji, J. F. R. Archilla, J. C. Eilbeck, and F. M. Russell, *Phys. Lett. A* **315**, 364 (2003).
- ¹²J. Cuevas, J. F. R. Archilla, B. Sanchez-Rey, and F. R. Romero, *Physica D* **216**, 115 (2006).
- ¹³A. V. Savin, E. A. Zubova, and L. I. Manevich, *Polym. Sci., Ser. A Ser. B* **47**, 376 (2005).
- ¹⁴W. Z. Chen, B. B. Hu, and H. Zhang, *Phys. Rev. B* **65**, 134302 (2002).
- ¹⁵A. Gavrielides, T. Kottos, V. Kovanis, and G. P. Tsironis, *Phys. Rev. E* **58**, 5529 (1998).
- ¹⁶B. Denardo, B. Galvin, A. Greenfield, A. Larraza, S. Putterman, and W. Wright, *Phys. Rev. Lett.* **68**, 1730 (1992).
- ¹⁷W. Z. Chen, *Phys. Rev. B* **49**, 15063 (1994).
- ¹⁸W. Z. Chen, Y. F. Zhu, and L. Lu, *Phys. Rev. B* **67**, 184301 (2003).
- ¹⁹W. Z. Chen, L. Lu, and Y. F. Zhu, *Phys. Rev. E* **71**, 036622 (2005).
- ²⁰H. Schiessel, G. Oshanin, A. M. Cazabat, and M. Moreau, *Phys. Rev. E* **66**, 056130 (2002).
- ²¹M. Kotrla, J. Krug, and P. Smilauer, *Phys. Rev. B* **62**, 2889 (2000).