Discrete breathers in a model with Morse potentials*

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Under harmonic approximation, this paper discusses the linear dispersion relation of the one-dimensional chain. The existence and evolution of discrete breathers in a general one-dimensional chain are analysed for two particular examples of soft (Morse) and hard (quartic) on-site potentials. The existence of discrete breathers in one-dimensional and two-dimensional Morse lattices is proved by using rotating wave approximation, local anharmonic approximation and a numerical method. The localization and amplitude of discrete breathers in the two-dimensional Morse lattice with on-site harmonic potentials correlate closely to the Morse parameter a and the on-site parameter κ.

Keywords: discrete breathers, Morse lattice, square lattice, on-site potential

PACC: 6320P, 6320R, 0547

1. Introduction

Since the discovery of intrinsic localized modes (ILMs) or discrete breathers (DBs) in Klein–Garden (KG) and Fermi–Pasta–Ulam (FPU) lattices in the late 1980s.[1,2] The DBs and solitons have been a topic of increasing focus in view of their significant roles in energy localization and transport. In 1994, Mackay and Aubry established the existence of stationary breathers in a broad range of models.[3] In their method, breathers are obtained by continuation from the anticontinuum limit at which the network is reduced to an array of uncoupled oscillators. Various properties of DBs or ILMs have been addressed theoretically,[4,5] i.e., DBs in one-dimensional (1D) mixed KG/FPU chain were studied by Zhou *et al.*[6] On the other hand, DBs have been recently observed experimentally in various physical contexts such as nonlinear photonic crystals,[7,8] superconducting Josephson-junction arrays,[9,10] and micromechanical cantilever systems.[11,12] Because the DBs' dynamics are similar to impurity modes that can move in gap, the discrete gap breathers (DGBs) as a kind of localized modes in 1D diatomic $\beta-$FPU chain, its local characteristic and stability were presented by Lü and Tian.[13,14] All of them mainly focused on 1D system. Recently, the DBs in the two-dimensional (2D) diatomic square lattice are increasingly catching people's interest. Possibilities of 2D DGBs have been discussed in a 2D diatomic face-centred square lattice,[15] and 2D DBs have also been discussed in FPU type,[16,17] sine-Gordon type lattices.[18] Yet it is unclear whether DBs exist in a more realistic lattice system. As mentioned by Sandusky and Page,[19] owing to the inclusion of the cubic anharmonicity, DBs cannot be generated in 1D monatomic lattices with realistic potentials of Lennard–Jones type. On the other hand, DBs can occur in such realistic lattices when the on-site potential is included.[20] In this case, the on-site potential plays a role of stabilizing localized structures. It seems that the detailed properties of DBs in higher-dimensional lattices with on-site potentials need to be further explored.

The purpose of this paper is to investigate the possibility of DBs in a 1D general model which are analysed for two particular examples of soft (Morse) and hard (quartic) on-site potentials. At the same time, we particularly pay attention to the DBs in a 2D Morse lattice with on-site harmonic potentials. This paper is organized as follows, in Section 2, under the harmonic approximation, we discuss the linearly dispersive relation of the phonon of a 1D model**.** Then, we introduce the basic equations of motion for a 1D monatomic chain. Some useful results of DBs in a 1D model are presented in this section. In Section 3, we analyse the numerical results, the generation, the evolution of 2D DBs and the various system parameters' effects on the 2D DBs in Morse lattice with on-site harmonic potentials. The paper is concluded by Section 4.

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2. Discrete breathers in 1D model

2.1. The linearly dispersive relation in 1D model

We consider a 1D chain of classical anharmonic oscillators (KG chain) (Fig. 1(a)) with Hamiltonian

$$H = \sum_{n=1}^{N}\left[\frac{1}{2}\dot{u}_n^2 + V(u_n) + \frac{1}{2}C_K(u_{n+1}-u_n)^2\right] = \sum_{n=1}^{N} H_n, \quad (1)$$

where the total energy attributed to each site n is defined as

$$H_n = \frac{1}{2}\dot{u}_n^2 + V(u_n) + \frac{1}{4}C_K[(u_{n+1}-u_n)^2 + (u_{n+1}-u_n)^2]. \quad (2)$$

The oscillators are submitted to a nonlinear on-site potential $V(u)$ and are coupled by a harmonic inter-site coupling $C_K > 0$. The nonlinear potential can be either a soft potential such as the Morse potential (Fig. 1(b))

$$V(u) = \frac{1}{2}\omega_0^2(\,\mathrm{e}^{-u}-1)^2, \quad (3)$$

or a hard potential such as the quartic potential (Fig. 1(c))

$$V(u) = \omega_0^2\left(\frac{1}{2}u^2 + \frac{1}{4}u^4\right). \quad (4)$$

(Recall that for a soft (hard) potential the oscillation frequency decreases (increases) with the oscillation amplitude or, equivalently, with the action). In the rest of the paper, we will consider $V''(0) = \omega_0^2 = 1$. The choice of the Morse potential is physically justified by the fact that it represents an appropriate description of hydrogen bonds, and it is then especially useful for the study of biological systems such as macromolecules and proteins. The equations of motion for the particle displacements u_n then take the form of a discrete nonlinear KG equation

$$\ddot{u}_n + V'(u_n) - C_K(u_{n+1}+u_{n-1}-2u_n) = 0. \quad (5)$$

For a given solution $u_n(\mathrm{t})$, the corresponding linearized equations are

$$\ddot{\varepsilon}_n + \varepsilon_n V''(u_n) - C_K(\varepsilon_{n+1}+\varepsilon_{n+1}-2\varepsilon_n) = 0, \quad (6)$$

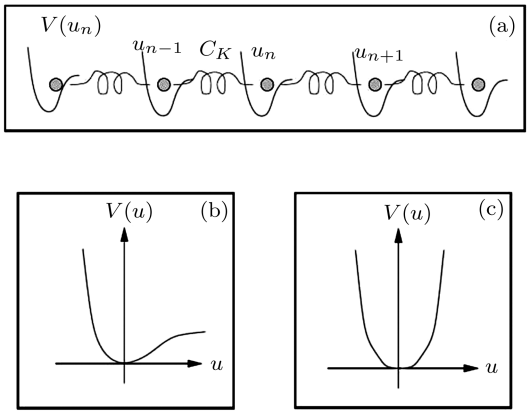


Fig. 1. (a) The KG chain of nonlinear oscillators with displacement $\{u\}$, coupled by a constant force C_K; (b) the soft Morse potential; (c) the hard quartic potential.

where ε_n denotes a small displacement with respect to the solution u_n. When $u_n = 0$ (or, more generally, when $V''(u_n)$ is constant), we obtain the standard harmonic (plane-wave) small-amplitude solutions

$$\varepsilon_n(t) = \varepsilon\cos(nQ - \omega_l(Q)t) \quad (7)$$

with wave vector Q and frequency $\omega_l(\mathrm{Q})$. By substituting these solutions in Eq. (6), we find the (phonon) dispersion relation

$$\omega_l^2(Q) = 1 + 4C_K\sin^2\frac{Q}{2} \quad (8)$$

for small-amplitude oscillations in a general potential.

2.2. The numerical results of discrete breathers in a generalized 1D chain

We consider a generalized discrete 1D monatomic chain, a system of atoms with unit mass, coupled anharmonically to their nearest neighbours and interacted with a nonlinear potential $V(u_n)$. The Hamiltonian of the system is given by

$$H = \sum\left[\frac{1}{2}\dot{u}_n^2 + V(u_n) + \frac{K_2}{2}(u_{n+1}-u_n)^2 + \frac{K_3}{3}(u_{n+1}-u_n)^3 + \frac{K_4}{4}(u_{n+1}-u_n)^4\right], \quad (9)$$

where u_n is the displacement of the n-th atom; K_2, K_3 and K_4 are the parameters controlling the strength of the nonlinear coupling, $V(u_n)$ is an on-site potential

$$V(u_n) = \frac{1}{2}\omega_0^2u_n^2 + \frac{1}{3}\alpha u_n^3 + \frac{1}{4}\beta u_n^4. \quad (10)$$

The equation of motion for the displacement of the n-th atom from its equilibrium reads as

$$\ddot{u}_n = -\omega_0^2u_n - \alpha u_n^2 - \beta u_n^3 + K_2(u_{n+1}+u_{n-1}-2u_n)$$

$$+ K_3\left[(u_{n+1}-u_n)^2-(u_n-u_{n-1})^2\right] + K_4\left[(u_{n+1}-u_n)^3-(u_n-u_{n-1})^3\right]. \quad (11)$$

The DBs are time periodic and spatially localized excitations. If they exist in the system and they are not propagating, they have the forms as follows:

$$u_n(t) = \Phi_n G(t), \quad (12)$$

where Φ_n corresponds to the spatial profile of the solution and $G(t)$ describes its time evolution. It is shown that this system has a class of solutions which can be written as a product of a purely spatial (n-dependent) part and a function of time only. Substituting Eq. (12) into Eq. (11) yields

$$\begin{aligned}&\left(\ddot{G}+\omega_0^2 G\right)\Phi_n \\ &= -\alpha G^2\Phi_n^2-\beta G^3\Phi_n^3-K_2\left(\Phi_{n+1}+\Phi_{n-1}+2\Phi_n\right)G \\ &\quad + K_3\left[(\Phi_{n+1}+\Phi_n)^2-(\Phi_n+\Phi_{n-1})^2\right]G^2 \\ &\quad - K_4\left[(\Phi_{n+1}+\Phi_n)^3+(\Phi_n+\Phi_{n-1})^3\right]G^3. \quad (13)\end{aligned}$$

The on-site anharmonic potential $V(u)$ can be expanded at the lowest significant order as

$$V(u) = \frac{1}{2}u^2+\alpha\frac{1}{3}u^3+\beta\frac{1}{4}u^4+\cdots. \quad (14)$$

For example, in the case of the hard quartic potential, the expansion yields $\alpha = 0$ and $\beta = 1$, while in the case of the Morse potential $\alpha = -3/2$ and $\beta = 7/6$. We can assume $G(t) = \cos\omega_b t$, so the solution $u_n(t)$ is written as $u_n(t) = \Phi_n \cos\omega_b t$. We seek for approximate solutions for DBs via the rotating wave approximation (RWA), local anharmonic approximation (LAA) and numerical method. We discuss the numerical results under two cases:

Case 1 The quartic on-site potential $\alpha = 0$ and $\beta = 1$

The equations of motion are given by

$$\begin{aligned}&\left(\omega_0^2-\omega_b^2\right)\Phi_n+\frac{1}{2}\beta\Phi_n^3+K_2\left(\Phi_{n+1}+\Phi_{n-1}+2\Phi_n\right) \\ &-\frac{\sqrt{2}}{2}K_3\left[(\Phi_{n+1}+\Phi_n)^2-(\Phi_n+\Phi_{n-1})^2\right] \\ &+\frac{1}{2}K_4\left[(\Phi_{n+1}+\Phi_n)^3+(\Phi_n+\Phi_{n-1})^3\right]=0. \quad (15)\end{aligned}$$

From the above numerical results, we prove the existence of DBs in 1D chains with quartic on-site potentials in Fig. 2(a). From Fig. 2(b), we can see the evolution of DBs with time in 1D chains with quartic on-site potentials.

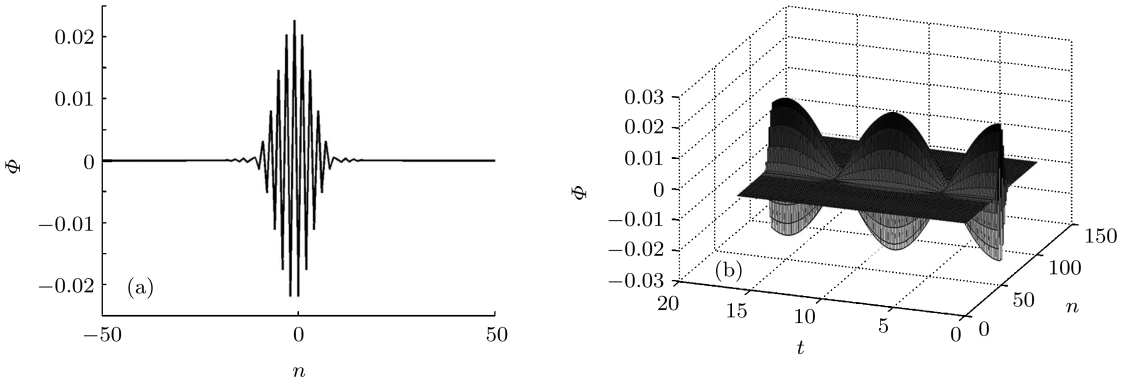


Fig. 2. Graphical illustration of the profiles of the DBs in 1D chains with quartic on-site potentials: (a) DBs are obtained numerically with $\beta = 1$, $K_2 = K_3 = K_4 = 1$; (b) the evolution of DBs with time.

Case 2 the Morse on-site potential $\alpha = -3/2$ and $\beta = 7/6$

The same as in the case 1, we still use RWA, LAA and numerical method to obtain the DBs in 1D chains with Morse on-site potentials. From the above numerical results, we proved the existence of DBs in 1D chains with Morse on-site potentials in Fig. 3(a). From Fig. 3(b), we can see the evolution of DBs with time in 1D chains with Morse on-site potentials. So, these numerical results prove the existence and evolution of DBs in a generalized 1D chain with quartic on-site potentials or Morse on-site potentials.

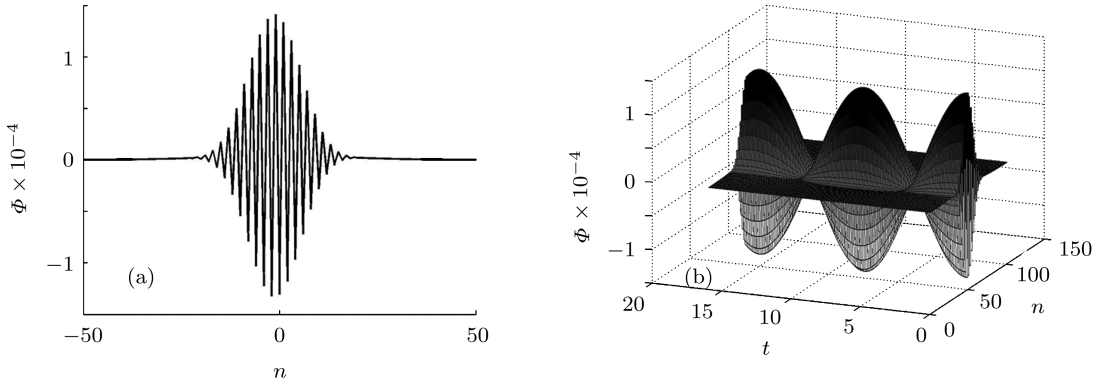


Fig. 3. Graphical illustration of the profiles of the 1D DBs in 1D chains with Morse on-site potentials: (a) DBs are obtained numerically with $\alpha = -3/2$ and $\beta = 7/6$, $K_2 = K_3 = K_4 = 1$; (b) the evolution of DBs with time.

3. Discrete breathers in a 2D square Morse lattice with on-site harmonic potentials

3.1. The numerical results of DBs in a 2D model

In this section, we discuss the DBs in a 2D Morse lattice with an on-site harmonic potential in terms of a square lattice of configuration. The interaction potential considered in this paper is the Morse potential given by

$$\Phi(r) = D[\,\mathrm{e}^{-2a(r-d)} - \mathrm{e}^{-a(r-d)}], \tag{16}$$

where r is the inter-particle distance, d is the equilibrium distance, and D is the minimum value of the potential function Φ. The potential parameter a represents the strength of nonlinearity of the Morse potential. At first, we consider a 1D monatomic lattice with nearest neighbour Morse interaction and on-site harmonic potentials. Thus, the equation of motion for the n-th particle is

$$m\ddot{q}_n = -f_n^{(r)} + f_{n-1}^{(r)} + f_n^{(q)}, \tag{17}$$

where the dot denotes the derivative with respect to time, $f_n^{(r)}$ is the interaction force between the n-th and the $(n+1)$-th particles due to the Morse potential in Eq. (16) and $f_n^{(q)}$ is the linear force due to the on-site harmonic potential, they are given by

$$\begin{aligned} f_n^{(r)} &= 2Da[\,\mathrm{e}^{-2a(r_n-d)} - \mathrm{e}^{-a(r_n-d)}], \\ f_n^{(q)} &= -\kappa(q_n - q_{n0}). \end{aligned} \tag{18}$$

Here $r_n = q_{n+1} - q_n$ denotes the relative displacement between the n-th and the $(n+1)$-th particle. The quantities in Eq. (17) can be nondimensionalized as

$$\begin{gathered} \hat{q}_n = q_n/d, \quad \hat{r}_n = r_n/d, \\ \hat{f}_n^{(r)} = (1/2Da^2) f_n^{(r)}, \\ \hat{f}_n^{(q)} = (1/2Da^2) f_n^{(q)}, \quad \hat{a} = da, \\ \hat{\kappa} = \kappa/2Da^2, \quad \hat{t} = \sqrt{2Da^2/m}\,t. \end{gathered}$$

Removing the hat from the nondimensional quantities leads to the following nondimensionalized equations:

$$\ddot{q}_n = -f_n^{(r)} + f_{n-1}^{(r)} + f_n^{(q)}, \tag{19}$$

$$\begin{aligned} f_n^{(r)} &= 2Da[\,\mathrm{e}^{-2a(r_n-1)} - \mathrm{e}^{-a(r_n-1)}], \\ f_n^{(q)} &= -\kappa(q_n - q_{n0}). \end{aligned} \tag{20}$$

Note that a is a nondimensional parameter measuring the strength of nonlinearity of the Morse potential and κ represents the strength of the on-site force. The 1D Morse lattice is extended to 2D case. Hence, the nondimensional equation of motion for the (n,m)-th particle is given by

$$\ddot{q} = \sum_{j=1}^{l} f_j^{(r)} + f^{(q)}, \tag{21}$$

$$\begin{aligned} f_j^{(r)} &= \frac{1}{a}\left[\mathrm{e}^{-2a(r_j-1)} - \mathrm{e}^{-a(r_j-1)}\right]\frac{\hat{r}_j}{r_j}, \\ f^{(q)} &= -\kappa(q - q_0), \end{aligned} \tag{22}$$

where $q \equiv q(n,m)$ is the displacement of the (n,m)-th particle, $r_j \equiv r_j\ (n,m)$ the relative displacement of the (n,m)-th particle with respect to the j-th neighbour particle, $r_j = |r_j|$ the corresponding magnitude, $f_j^{(r)}$ is the interaction force between the (n,m)-th particle and the j-th particle, and $f^{(q)}$ is the on-site linear force.

In the following, we seek for approximate solutions for DBs via RWA, LAA and numerical method. It is easily shown that the Morse potential admits a Taylor expansion:

$$f_j^{(r)} = \frac{1}{a}\left[\mathrm{e}^{-2a(r_j-1)} - \mathrm{e}^{-a(r_j-1)}\right]\frac{\hat{r}_j}{r_j} = \left[-(r_j-1)+\frac{3}{2}a(r_j-1)^2 - \frac{7}{6}a^2(r_j-1)^3+\cdots\right]\frac{\hat{r}_j}{r_j}. \quad (23)$$

In a square lattice, we assume that the solution of the equation of motion is $u_{n,m} = u^0_{n,m}G(t)$, where $u^0_{n,m}$ corresponds to the spatial profile of the solution and $G(t)$ describes its time evolution. For the square lattice, we label as $(n+1,\ m)$, $(n,\ m+1)$, $(n-1,\ m)$, $(n,\ m-1)$ the nearest neighbouring four particles and $(n+1,\ m+1)$, $(n-1,\ m+1)$, $(n-1,\ m-1)$, $(n+1,\ m-1)$ the second nearest neighbouring four particles. From Eqs. (21), (22) and (23), considering the interactions with the nearest and second nearest neighbouring particles, we obtain the spatial equation of motion as follows:

$$\begin{aligned}
&(u^0_{n+1,m}+u^0_{n-1,m}+u^0_{n,m+1}+u^0_{n,m-1}-4u^0_{n,m})+(u^0_{n+1,m+1}+u^0_{n-1,m-1}-u^0_{n+1,m-1}-u^0_{n-1,m+1}-4u^0_{n,m})\\
&+\frac{3}{2}a\left[\left(u^0_{n+1,m}-u^0_{n,m}\right)^2-\left(u^0_{n,m}-u^0_{n-1,m}\right)^2+\left(u^0_{n,m+1}-u^0_{n,m}\right)^2-\left(u^0_{n,m}-u^0_{n,m-1}\right)^2\right]\\
&+\frac{3}{2}a\left[\left(u^0_{n+1,m+1}-u^0_{n,m}\right)^2-\left(u^0_{n,m}-u^0_{n-1,m-1}\right)^2+\left(u^0_{n+1,m-1}-u^0_{n,m}\right)^2-\left(u^0_{n,m}-u^0_{n-1,m+1}\right)^2\right]\\
&-\frac{7}{6}a^2\left[\left(u^0_{n+1,m}-u^0_{n,m}\right)^3-\left(u^0_{n,m}-u^0_{n-1,m}\right)^3+\left(u^0_{n,m+1}-u^0_{n,m}\right)^3-\left(u^0_{n,m}-u^0_{n,m-1}\right)^3\right]\\
&-\frac{7}{6}a^2\left[\left(u^0_{n+1,m+1}-u^0_{n,m}\right)^3-\left(u^0_{n,m}-u^0_{n-1,m-1}\right)^3+\left(u^0_{n+1,m-1}-u^0_{n,m}\right)^3-\left(u^0_{n,m}-u^0_{n-1,m+1}\right)^3\right]\\
&-\kappa u^0_{n,m}=0. \quad (24)
\end{aligned}$$

From the above equation of motion, we prove the existence of DBs in a square lattice by using RWA, LAA and the numerical method. According to the following numerical results, we know that the existence of the 2D DBs in a 2D square Morse lattice is possible. The 2D DBs have the following three cases to analyse because of various effects of the system parameters. We apply symmetric excited pattern and asymmetric excited pattern by using numerical calculation. We also investigate the relation between the 2D DBs profile and Morse potential parameter a and the on-site potential parameter κ by comparing Fig. 4 with Figs. 5 and 6.

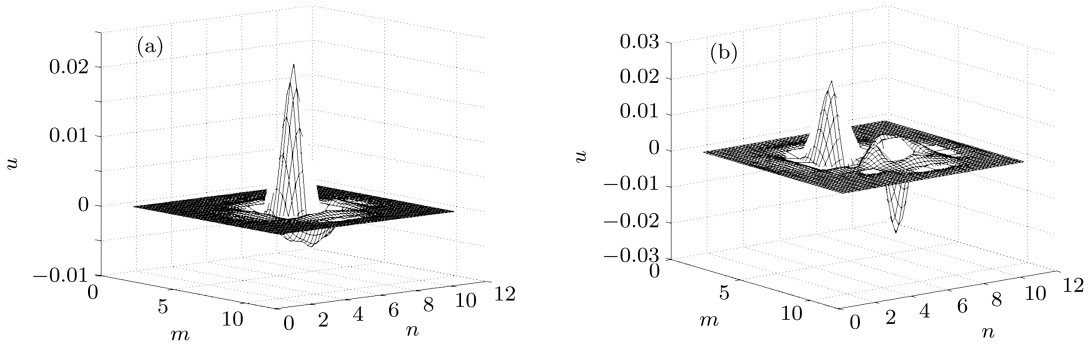


Fig. 4. Graphical illustration of the profiles of the 2D DBs in 2D monatomic square lattice: (a) the symmetric pattern obtained numerically with $a = 1$, $\kappa = 1$; (b) the asymmetric pattern obtained numerically with $a = 1$, $\kappa = 1$.

(i) We assign smaller values to a and κ, the numerical results of 2D DBs are shown in Fig. 4.

(ii) We assign larger values to a and κ, the numerical results of 2D DBs are shown in Fig. 5.

By comparing Fig. 5 with Fig. 4, we find that the larger the parameters a and κ, the better localization of the 2D DBs profile. The larger the parameters a and κ, the larger the amplitude of the 2D DBs.

(iii) We assign a smaller value to a and a larger value to κ, the numerical results of 2D DBs are shown in Fig. 6.

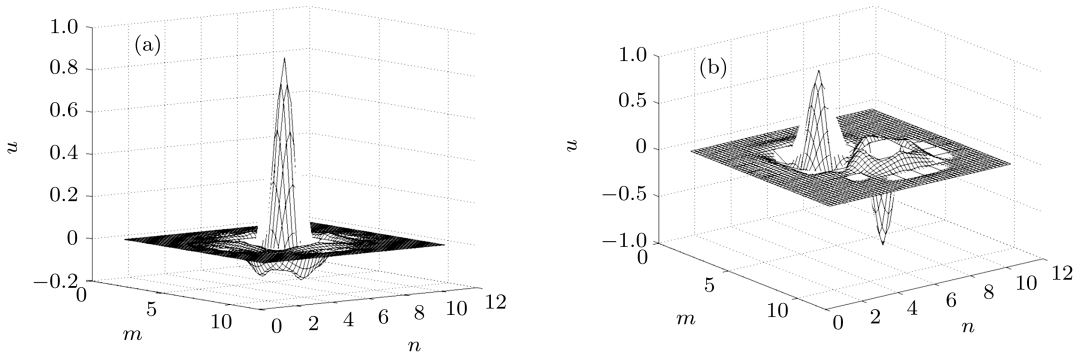


Fig. 5. (a) The symmetric pattern with $a = 10$, $\kappa = 10$; (b) the asymmetric pattern with $a = 10$, $\kappa = 10$.

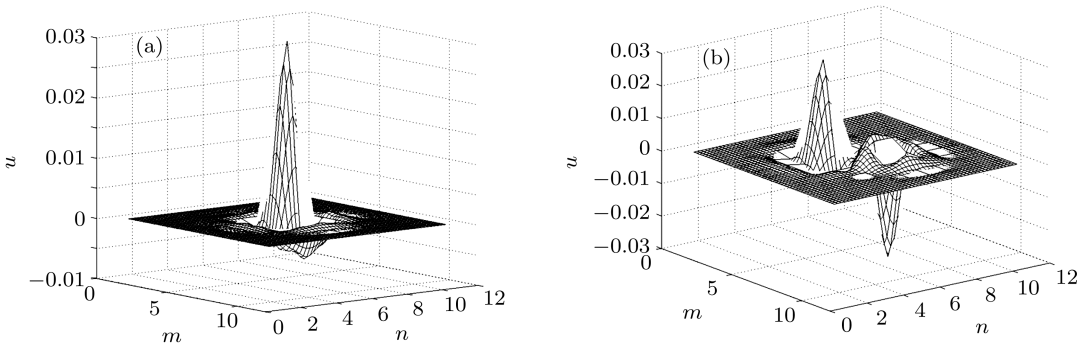


Fig. 6. (a) The symmetric pattern with $a = 1$, $\kappa = 10$; (b) the asymmetric pattern with $a = 1$, $\kappa = 10$.

By comparing Fig. 6 with Fig. 4, the above results show that on-site potential parameter κ plays an important role in the amplitude and localization of DBs in 2D square Morse lattice with on-site harmonic potentials.

3.2. Summary of results for the 2D square Morse lattice with on-site harmonic potentials

Various numerical simulations are performed by varying the parameters a, κ. The properties of DBs in 2D square Morse lattice with on-site harmonic potentials are summarized as follows:

(I) When the on-site harmonic potentials κ are included in the Morse model, the on-site linear force has the effect of generating and stabilizing localized modes. The localization tends to arise when the effect of the on-site potential becomes significant, which can be explained by a fact that a larger κ means a larger restoring force to maintain staggering oscillations.

(II) A large value of the potential parameter a implies a strong nonlinearity of the interaction potential. This fact indicates that if 2D localization is possible, its solution should be very sharp and highly localized, in which only a few particles get involved in the oscillation. Such highly localized 2D modes are usually unstable. However, if the on-site force becomes significant, quasi-one-dimensional localization (a 1D-mode) becomes possible. Particles are highly localized in one direction but the on-site force can induce localized oscillations of several particles along another direction. This is a qualitative interpretation for the results of 2D-modes.

(III) It seems that there exists an upper limit for the amplitude of generated DBs in 2D lattice. We think that they are apt to be unstable because of an additional degree of freedom. These results show that the evolution processes (i.e., generation of DBs and their evolution) differ from the 1D lattice case. Because of the extra degree of freedom, generated localized modes tend to be unstable and are more easily

destroyed by disturbance.

4. Conclusions

In this paper, we mainly investigated the possibility of DBs in a 1D general model which are analysed for two particular examples of soft (Morse) and hard (quartic) on-site potentials. At the same time, we particularly pay attention to the DBs in 2D Morse lattices with on-site harmonic potentials. Under the harmonic approximation, we discussed the linearly dispersive relation of the phonon of a 1D model. Numerical results for the approximate DBs, the generation and the evolution of DBs in a 1D generalized model are presented in this passage, we proved their existence by using RWA, LAA and the numerical method. Applying the same method, we analysed the numerical results in the 2D system. We attained the conclusions that the larger Morse potentials and on-site harmonic potentials, the better localization of the 2D DBs' profiles and the larger amplitude of the 2D DBs. A large value of the potential parameter a implies a strong nonlinearity of the interaction, the highly localized 2D modes are usually unstable. However, if the on-site force becomes significant, quasi-one-dimensional localization (a 1D-mode) becomes possible. Particles are highly localized in one direction but the on-site force can induce localized oscillations of several particles along another direction. Additionally, in a 2D Morse lattice with on-site harmonic potentials, the on-site potential κ plays an important role in the amplitude and stability of DBs. The localization of 2D DBs tends to arise when the effect of the on-site potential becomes significant, which can be explained by the fact that a larger κ means a larger restoring force to maintain staggering oscillations. But there exists an upper limit for the amplitude of generated DBs in 2D lattices. We think that they are apt to be unstable because of an additional degree of freedom.

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