Structures of Discrete Breathers in Two-Dimensional Fermi-Pasta-Ulam Lattices

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Discrete breathers (DBs) or intrinsic localized modes (ILMs) are energy localization in nonlinear lattice systems. One of the characteristic properties of DB is that they can be excited even in higher dimensional systems. Indeed, it has been reported that DB can be formed in two dimensional lattice systems as a result of energy concentration from some perturbations. However detailed studies of DBs in the higher dimensional system have not been done yet. In this paper, we investigate structures and dynamics of quasi-one dimensional DBs in two dimensional Fermi-Pasta-Ulam (FPU) lattice systems.

1. INTRODUCTION

Localized structures in nonlinear lattice systems called discrete breathers (DBs) or intrinsic localized modes (ILMs) have attracted much attention since the first report by Sievers and Takeno in 1988.1 DB is a time-periodic and space-localized structure which is excited due to both discreteness and nonlinearity of the systems. These two factors lead characteristic properties of DBs: (i) higher angular frequencies than those of the linear plane waves (phonon mode), (ii) zig-zag displacement of particles. Various studies on statical and dynamical properties of DBs have been done both theoretically and numerically in the past decades.2-4 Recently observations of DBs in the real physical systems have been reported: locked and moving ILMs on micromechanical cantilever arrays,3 localization of lasers in waveguide arrays4 and localized structures in superconducting Josephson-junction arrays.5,6 The observations of DBs in the various experiments indicate the importance of the study of DBs in the realistic situations.

One of the most interesting examples of realistic lattice systems is crystal lattice structure. In this structure, atom or molecule are spaced periodically. They are connected through interaction potential. In general, this interaction potential has nonlinearity. Therefore DB can be excited as the atomic scale vibration in the crystal lattice structures.

While most of the studies on DBs have been done in ideal systems like the one dimensional Fermi-Pasta-Ulam (FPU) lattices, some studies have been done in the view of DB’s application to dynamics of atoms in the crystal lattice structure. In these studies, one of the most important factors considerations of the realistic properties of the interaction potentials: an asymmetric shape and a soft potential. For example, Bickham et al investigated the effect of asymmetry of the interaction potential on the shape of DBs in the system with the cubic and quartic anharmonicity.7 They showed that the shape of DBs is deformed by the excitation of the lattice distortion called DC effect and that too large cubic anharmonicity leads to collapse of DB.
Another important consideration is the dimension of the systems. It has been shown that DB can exist in the higher dimensional systems than one dimensional one.\textsuperscript{9} For example, it has been reported that DB can be excited in the two dimensional systems\textsuperscript{9} and the edge of the three dimensional system.\textsuperscript{10} Marín\textsuperscript{9} et al have showed that a moving DB is excited from the large initial displacement of neighboring three particles in the hexagonal lattice system with Lennard-Jones potential. It is expected that increasing of the number of degrees of freedom per particle leads various localized structures than those in the one dimensional systems. Ikeda has reported that there are two types of DB, that is, quasi-one dimensional and two dimensional DBs, in the two dimensional systems with Morse potential and harmonic on-site potentials.\textsuperscript{11} However none of accurate structures of DBs even in the perfect two dimensional lattices have been investigated either theoretically or numerically.

In this paper, we investigate the structures of DB in the two dimensional FPU type square lattices. We focus on the quasi-one dimensional DBs in the system. We show that the structure and the angular frequency of DB are affected by the structure of the lattice system.

2. MODELS

2.1 EQUATIONS OF MOTION

As mentioned above, we consider the two dimensional FPU-type square lattice system. Figure 1 shows the model of the two dimensional square lattice system. Particles are arranged periodically in both the $x$ and $y$ directions. Each particle is connected to their nearest and second nearest neighbor particles through the interaction potential. Hamiltonian of the system is given by,

$$
H = \sum_{i,j} \frac{1}{2} \dot{x}_{ij}^2 + \sum_{i,j} \left[ V(x_{ij}, x_{i+1,j}, d_1) + V(x_{ij}, x_{i,j+1}, d_1) \right] + \alpha \sum_{i,j} \left[ V(x_{ij}, x_{i+1,j+1}, d_2) + V(x_{ij}, x_{i-1,j+1}, d_2) \right],
$$

where $x_{ij} = (x_{i,j}, y_{i,j})$ is the position vector of the $(i, j)$-th particle. $d_1$ and $d_2$ are the distances to the nearest and the second nearest neighbor particles in equilibrium, respectively. $\alpha$ indicates strength of the interaction with the second nearest neighbor particles. We can set $d_1 = 1$ without loss of generality. The interaction potential $V$ is given by,

$$
V(x_1, x_2, d) = v(|x_1 - x_2| - d),
$$

$$
v(r) = \frac{1}{2} r^2 + \frac{1}{4} \beta r^4,
$$

where $\beta$ is the quartic anharmonic parameter of the system.

From eq.(1), we can obtain the equations of motion of each particle as follows,

$$
\frac{d^2 x_{i,j}}{dt^2} = F(x_{ij}, x_{i+1,j}, 1) + F(x_{ij}, x_{i-1,j}, 1) + F(x_{ij}, x_{i,j+1}, 1) + F(x_{ij}, x_{i,j-1}, 1) + \alpha F(x_{ij}, x_{i,j+1}, d_2) + \alpha F(x_{ij}, x_{i,j-1}, d_2) + \alpha F(x_{ij}, x_{i+1,j+1}, d_2) + \alpha F(x_{ij}, x_{i-1,j+1}, d_2).
$$
Function $F$ denotes force which act between two particles at $x_1$ and $x_2$,

$$F(x_1, x_2, d) = -f(|x_2 - x_1| - d) \frac{x_2 - x_1}{|x_2 - x_1|},$$  \hspace{1cm} (5)$$

$$f(r) = r + \beta r^3.$$  \hspace{1cm} (6)$$

2.2 LINEAR DISPERSION RELATION

For the following discussion, we derive the linear dispersion relation of the system (1). At first, we introduce new variables $\tilde{x}_{i,j}$ and $\tilde{y}_{i,j}$ which indicate the displacements from equilibrium point in the $x$ and $y$ directions, respectively:

$$x_{i,j} = \tilde{x}_{i,j} + i,$$

$$y_{i,j} = \tilde{y}_{i,j} + j.$$  \hspace{1cm} (7)$$

(8)$$

Suppose $\tilde{x}_{i,j}$ and $\tilde{y}_{i,j}$ are small and substituting expressions (7) and (8) into eqs.(4), the linearized equations of motion are derived as follows,

$$\frac{d^2 \tilde{x}_{i,j}}{dt^2} = A(\tilde{x}_{i-1,j-1} + \tilde{x}_{i-1,j+1} + \tilde{x}_{i+1,j-1} + \tilde{x}_{i+1,j+1}) + \tilde{x}_{i+1,j} + \tilde{x}_{i-1,j} - 2(1 + 2A)\tilde{x}_{i,j}$$

$$+ B(\tilde{y}_{i-1,j-1} - \tilde{y}_{i-1,j+1} - \tilde{y}_{i+1,j-1} + \tilde{y}_{i+1,j+1}),$$  \hspace{1cm} (9)$$

$$\frac{d^2 \tilde{y}_{i,j}}{dt^2} = A(\tilde{y}_{i-1,j-1} + \tilde{y}_{i-1,j+1} + \tilde{y}_{i+1,j-1} + \tilde{y}_{i+1,j+1}) + \tilde{y}_{i,j-1} + \tilde{y}_{i,j+1} - 2(1 + 2A)\tilde{y}_{i,j}$$

$$+ B(\tilde{x}_{i-1,j-1} - \tilde{x}_{i-1,j+1} - \tilde{x}_{i+1,j-1} + \tilde{x}_{i+1,j+1}),$$  \hspace{1cm} (10)$$

where $A$ and $B$ are constants and defined as,

$$A = \frac{\alpha}{4}(4 - \sqrt{2d_2} + 16\beta - 18\sqrt{2d_2\beta} + 12d_2\beta - \sqrt{2d_2^3\beta}),$$  \hspace{1cm} (11)$$

$$B = \frac{\alpha}{4}(\sqrt{2d_2} + 8\beta - 6\sqrt{2d_2\beta} + \sqrt{2d_2^3\beta}).$$  \hspace{1cm} (12)$$
By substituting
\[ \tilde{x}_{m,n} = X \exp [i(km + ln - \omega t)], \]
\[ \tilde{y}_{m,n} = Y \exp [i(km + ln - \omega t)], \]
into eqs.(9) and (10), we obtain two branches of the linear dispersion relation
\[ \omega^2_x = -4A \cos k \cos l + 2(1 + 2A) - (\cos k + \cos l) + \sqrt{(\cos k - \cos l)^2 + 16B^2 \sin^2 k \sin^2 l}, \]
\[ \omega^2_y = -4A \cos k \cos l + 2(1 + 2A) - (\cos k + \cos l) - \sqrt{(\cos k - \cos l)^2 + 16B^2 \sin^2 k \sin^2 l}. \]
(15)

where \( k \) and \( l \) are wave number along the \( x \) and \( y \) directions. Wave vector is defined by \( k = (k, l) \).

Figure 2 shows the linear dispersion curve of the values of the parameters \( \alpha = 1.0, \beta = 4.0 \)
and \( d_2 = 1.0 \) along the lines in \( k \)-space as follows:

\[
(k, l) = \begin{cases} 
(k_1, 0) & (0 < k_1 < \pi) \quad O \rightarrow A \\
(\pi, l_1) & (0 < l_1 < \pi) \quad A \rightarrow B \\
(k_2, 0) & (0 < k < \pi) \quad B \rightarrow O 
\end{cases} \tag{16}
\]

Two branches of phonon modes have different pairs of the \( X = (X, Y) \) in eqs. (13) and (14) as follows,

\[
(X, Y) = \begin{cases} 
(C_{1+}, 0) & : \omega_+ \\
(C_{2+}, 0) & : \omega_+ \\
(C_{3+}, C_{3+}) & : \omega_+ \\
(C_{3-}, -C_{3-}) & : \omega_- \\
(0, C_{1-}) & : \omega_- \\
(0, C_{2-}) & : \omega_- \\
(C_{3-, C_{3+}}) & : \omega_- \\
(C_{3-, C_{3+}}) & : \omega_- 
\end{cases} \tag{17}
\]

where \( C_{m+} \) and \( C_{n-} \) are constant values. Therefore two branches have different displacement pattern of particles. Especially, in the first case cases of \( (O \rightarrow A) \) and the third case \( (B \rightarrow O) \),
the phonon modes \( \omega_+ \) and \( \omega_- \) correspond to the longitudinal wave and the transverse wave, respectively, because of \( X_+ \parallel k, X_- \perp k \).

Angular frequency \( \omega \) is maximized in the case of the longitudinal wave with \( k = \pi, l = 0 \) or \( k = 0, l = \pi \). Maximum angular frequency \( \omega_{\text{max}} \) is
\[ \omega_{\text{max}}^2 = 4(1 + 2A). \tag{18} \]

Figure 3 shows the displacement pattern of particles of the phonon mode with the maximum angular frequency \( \omega_{\text{max}} \). In these cases, the system has zig-zag displacement along to one direction (the direction of \( K \)) and uniform displacement along to the other direction.

Next we see the relation between \( \omega_{\text{max}} \) and the parameters of the system: the distance to the effect of the interaction with the second nearest neighbor particle \( \alpha \), the second nearest neighbor particles in equilibrium \( d_2 \) and the nonlinearity of the system \( \beta \). Figure 4 shows these relations. We can see the following facts:

1. As \( \alpha \) becomes larger, \( \omega_{\text{max}} \) becomes larger
2. As \( d_2 \) become smaller, \( \omega_{\text{max}} \) becomes larger.
3. The linear dispersion relation depends on the nonlinear parameter \( \beta \) when \( d_2 \neq \sqrt{2} \).
Figure 2: Linear dispersion relation of the model (1) with $\alpha = 1.0$, $\beta = 4.0$ and $d_2 = 1.0$. Solid and dashed line indicates two branches of phonon mode $\omega_1$ and $\omega_2$, respectively. Right panel indicates the path in the $k$-space.

Figure 3: Displacement pattern of particles in the case for maximum angular frequency.

Figure 4: Parameter dependency on the maximum angular frequency $\omega_{\text{max}}$: (a) parameter of second nearest neighbor interaction $\alpha$ ($\beta = 4.0$, $d_2 = 1.0$), (b) nonlinear parameter $\beta$ ($\alpha = 1.0$) and (c) equilibrium distance between second nearest neighbor particles $d_2$ ($\alpha = 1.0$).

3. NUMERICAL CALCULATION

Since DB is the time-periodic solution, it takes the periodic orbits in the phase space. Its angular frequency is higher than the maximum angular frequency of the linear dispersion relation $\omega_{\text{max}}$. Suppose the function $G$ describes the temporal evolution of $X_0$ in the phase space, we can write as follows:

$$X(t) = G(t, X_0).$$  \hspace{1cm} (19)

If the point $X_{\text{DB}}$ is on the periodic orbit which corresponds to the DB with the angular frequency $\omega_{\text{DB}}$, following relation should be satisfied,

$$X_{\text{DB}}(t) = X_{\text{DB}} \left( t + n \frac{2\pi}{\omega_{\text{DB}}} \right) \quad n: \text{integer},$$  \hspace{1cm} (20)

From eqs. (19) and (20), $X_{\text{DB}}$ should satisfy the following equation,

$$G \left( \frac{2\pi}{\omega_{\text{DB}}}, X_{\text{DB}} \right) - X_{\text{DB}} = 0.$$  \hspace{1cm} (21)
Finding the DB with the angular frequency $\omega_{\text{DB}}$ is nothing but solving eq. (21). We try to find the numerical solution of eq. (21) by the Newton-Raphson method. Note that we have to calculate the function $G$ numerically by integrating of eqs.(4), because $G$ in not given in the analytical form. In this paper, we use the 6th order symplectic integration scheme for numerical integration.

4. NUMERICAL RESULTS

We calculate the DBs in the two dimensional lattice system with $20 \times 21$ particles. Fixed boundary conditions are considered. Time step $\Delta t$ in numerical integrations for obtaining the periodic orbits are determined by

$$\Delta t = T_{\text{DB}} = \frac{2\pi}{\omega_{\text{DB}} N_{\text{step}}}.$$  \hspace{1cm} (22)

We set $N_{\text{step}} = 5000$.

Then we search the periodic orbits with the angular frequency $\omega_{\text{DB}}$. At first, we use the approximated solutions as the trial solution for the Newton-Raphson method. The approximated solution are calculated in the case that only three particles are excited as DB in the one dimensional system with interaction only to nearest neighbor particle.

Once we obtain the numerical solution for the specific condition $(\bar{\omega}_{\text{DB}}, \bar{\alpha}, \bar{d}_2, \bar{\beta})$, we use this conditions as the trial solution of next Newton-Raphson method for the conditions in which the parameters are varied a bit, i.e., from $(\bar{\omega}_{\text{DB}}, \bar{\alpha}, \bar{d}_2, \bar{\beta})$ to $(\bar{\omega}_{\text{DB}} + \delta\omega_{\text{DB}}, \bar{\alpha}, \bar{d}_2, \bar{\beta})$. We continue this procedure until we reach the goal $(\omega_{\text{DB}}, \alpha, \bar{d}_2, \beta)$.

Figure 5 shows the numerical solutions of the quasi-one dimensional DB. Top panels in each figure indicate the displacement pattern in the two dimensional plane. Bottom panels indicate the displacements of the particles $x_{i,0}$ and $x_{i,1}$ in the $x$ direction. Obtained DBs have structures which corresponding to the longitudinal vibrations, that is, direction of particle’s vibration is parallel to the wave vector $k$. And DBs are stationary ones whose peak of envelope does not move in the system. Each particle in the stationary DB vibrates with the angular frequency $\omega_{\text{DB}}$ with keeping DB's zig-zag displacement. Adding to this, it is found that as the angular frequency $\omega_{\text{DB}}$ becomes larger, the amplitude and the localization become larger.

Figure 5(a) shows the solution without the interaction with the second nearest neighbor particles ($\alpha = 0$). In this case, localized structure excited only on the line of $j = 0$. Displacement along the $y$ direction is not excited. Therefore the system without interaction with the second nearest neighbor particles can be regarded as one dimensional lattice system with on-site potential. Effects of the two dimensional lattice only appear as the on-site effect of lines $j = 0$.

Figures 5(b) and (c) indicate the solutions with second nearest neighbor interactions ($\alpha = 1.0, d_2 = 1.0$). Figure 5(b) and (c) are shown for the cases for the low $\omega_{\text{DB}} = 2.4$ and high angular frequency $\omega_{\text{DB}} = 4.2$, respectively. Amplitude of the DB with the higher angular frequency is larger than DB with the lower angular frequency. In these cases, displacement of particles is observed not only on line $j = 0$, but also on line $j = 1$ (and $j = -1$). Especially, in the case for the small amplitude, amplitude of particles on $j = 1$ (and $j = -1$) is almost equal to that on $j = 0$. And we can see that particles take the anti-phase (zig-zag) displacement along the $x$ direction. For the $y$ direction, on the other hand, they take the in-phase (uniform) displacement. This difference of the displacement pattern between the $x$ and $y$ directions is the
same as that of the phonon mode for the maximum angular frequency $\omega_{\text{max}}$ which are shown in the left panel of figure 3.

Another significant effect of the second nearest neighbor interaction on the structure of DB is the break of the symmetry of DB. In the case for $\alpha = 0$, DB has mirror symmetry on the peak of localization. However, in the case for $\alpha \neq 0$, this symmetry is lost. This break of the symmetry becomes more significant as the equilibrium distance $d_2$ becomes smaller. Similar break of DB’s symmetry is also observed in the one dimensional lattice system with the asymmetric potentials. This similarity indicates that the second nearest interactions act a asymmetric effect on quasi-one dimensional DBs, because direction of the particle displacement is different form that of force to the second nearest particles.

Finally, the effect of second nearest neighbor interaction on the angular frequency $\omega_{\text{DB}}$ are considered. Figure 6 shows the these relations. The angular frequency $\omega_{\text{DB}}$ is above on upper bound of the linear dispersion relation (18). As seen in section 2.2, $\omega_{\text{max}}$ becomes larger as $d_2$ becomes smaller. Therefore $\omega_{\text{DB}}$ becomes larger when $d_2$ becomes smaller.

5. CONCLUDING REMARKS

In this paper, we investigate the structure of DBs in the two dimensional anharmonic lattice systems. The quasi-one dimensional DBs are obtained by means of the Newton-Raphson method. And we find that DB’s dynamical properties are affected by introducing the interaction with the second nearest neighbor particle: the deformation of DBs shape and the larger angular frequency. These facts indicate that more complex dynamics of DBs in the two dimensional systems than that in the one dimensional systems. Finally we point out problems for future investigations: (i) stability analysis of the DBs in the two dimensional systems, (ii) numerical analysis for another types of DBs and (iii) study on the moving DBs in the two dimensional systems.
Figure 6: Relation between the angular frequency \( \omega_{DB} \) and the amplitude of DBs for \( \alpha = 0 \) and \( \beta = 4.0 \). Perpendicular lines indicate \( \omega_{\text{max}} \) for each case.

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