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Head-on and head-off collisions of discrete breathers in two-dimensional anharmonic crystal lattices

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Abstract. Collisions of discrete breathers (DB) moving toward each other along neighboring close packed atomic rows in a 2D crystal lattice are investigated by molecular dynamics computer simulations. It is shown that a DB can draw energy from the other and emerge from the collision with amplitude much greater than its initial amplitude.

1 Introduction

There is not doubt that the theoretical discovery [1,2] and subsequent experimental observation of selftrapped localized modes or intrinsic localized modes (ILM) aka discrete breathers (DB) in nonlinear perfect (defect-free) crystal lattices a few decades ago [3–10] was a milestone in Physics. This happened two decades after the discovery of the soliton in continuous and anharmonic lattice systems [11–13]. Although one could provide a mathematical framework where both concepts could be placed together in a single, common definition, this would hide significant differences between solitons and DB [14–25]. Firstly, although DB appear as lattice excitations which are (typically exponentially) localized over a limited range of lattice sites and decay to zero far from these, and are temporally periodic, they are not an analog of the solitons in continuous media nor they are lattice solitons [11–13]. Secondly, solitons originate in the study of integrable nonlinear partial differential equations like the paradigmatic Boussinesq-Korteweg-de Vries (BKdV) equation. They also appear in the study of longitudinal vibrations, acoustic modes in anharmonic lattices like in the Toda lattice. In the latter case no on-site potential exists and only intersite potentials are considered. DB generally come from non-integrable systems. Solitons may appear either as localized, single pulse excitations embracing a few lattice sites or as periodic waves like the cnoidal waves of the BKdV equation. In such paradigmatic cases (BKdV, Toda) they are the result of, e.g., the dynamic balance between nonlinearity and dispersion but this need not to be always the case. DB seem to be a consequence of nonlinearity and lattice discretness, with strong enough on-site potentials and intersite potentials playing a minor albeit significant role at least in 1D systems. This need not to be so in higher dimensions like in a 2D crystal lattice. There is the argument that localized vibrations in perfectly periodic (defect-free) non-integrable lattices can be "de facto" stabilized by lattice discretness which provides a natural habitat for vibrational energy localization. A curious feature is that lattice sites, call them atoms or particles, inside a DB with different amplitudes vibrate all with the same frequency though separately in nonlinear oscillations the frequency depends on amplitude. Besides DB seem to easily occur in any dimension while genuine lattice solitons may have difficulties to survive with generality.

The coinage of the concept of soliton by Zabusky and Kruskal [11] comes from the apparent particle-like behavior of colliding solitary waves (in their BKdV case when overtaking). Solitons offer well-defined signatures when colliding head-on, overtaking or traveling in oblique directions. Noteworthy is that upon collision solitons behave kinematically very much like shocks which exist due to the dynamic balance between nonlinearity and dissipation. Finally, lattice solitons like in the Toda case are always supersonically moving localized excitations whereas DB are either pinned or if moving they seem not to become supersonic.

DB do not radiate their energy in the form of small-amplitude waves because they vibrate at frequencies outside the phonon spectrum of the crystal. The DB frequency can leave the phonon spectrum when its amplitude is sufficiently large because the frequency of a nonlinear oscillator is amplitude-dependent. For a hard-type anharmonicity the frequency increases with amplitude and it can grow above the phonon spectrum [26,27]. For a soft-type anharmonicity the frequency of a nonlinear mode decreases with amplitude and such mode can exist only

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if the phonon spectrum possesses a gap. As in crystals is far from easy to realize a hard-type anharmonic vibrational mode most of the studies were devoted to the analysis of gap DB exhibiting the soft-type anharmonicity [28–38]. Nevertheless DB with frequencies above the phonon spectrum have been identified in Si and Ge [26] and more recently in pure metals such as fcc Ni and bcc Nb [27].

In the 80s Campbell et al. published results on the resonant kink-antikink collisions in the ϕ^4 and double-sine-Gordon models when they can merge into a breather or escape [39–41]. Collisions between two breathers in a weakly perturbed sine-Gordon field were analyzed [42]. DB can emerge as a result of modulational instability in 1D, 2D and 3D lattices [43–47]. In the far-from-equilibrium conditions, when only one or a few short-wavelength extended waves are excited, larger DB grow by harvesting energy from smaller DB. The definition of moving DB has been given in [15,48]. The possibility of energy exchange between colliding DB and merger of two colliding DB have been demonstrated in [49,50].

Well-localized DB, having frequencies well apart the phonon band edges, must have large enough amplitudes. It is thus of interest to understand possible mechanisms of energy gain by DB. In the present study, using a suitable ansatz to excite moving DB with hard-type anharmonicity in a 2D crystal, collisions of such DB are analyzed numerically. Little is known about head-off collisions of DB which are possible in 2D, when two DB approach each other moving along parallel lines.

We would like to see the signatures of head-on and head-off DB collisions and observe basic similarities and differences with respect to soliton collisions in order to illuminate experimenters in their search for applications [51–63].

2 Simulation setup and properties of discrete breathers

A two-dimensional (2D) close packed lattice with the interatomic distance (lattice constant) equal to a is considered. Intersite interactions are described by the empirical Morse potential

$$U(r) = D(e^{-2\alpha(r-r_m)} - 2e^{-\alpha(r-r_m)}), \qquad (1)$$

where r is the distance between two atoms, D, α, r_m are the potential parameters. The function $U(r)$ has a minimum at $r = r_m$, the depth of the potential (the binding energy) is equal to D and α defines the stiffness of the bond. In the following, we choose scales of time, energy and distance such that $D = 1$, $r_m = 1$ and the atom mass is unity. We take $\alpha = 5$, for which the equilibrium interatomic distance is $a = 0.98813$. The cut-off radius is chosen to be $r_c = 5$. Due to the long-range interaction $a < r_m$.

The computational cell, generated by the translation vectors $\mathbf{a}_1 = a(1, 0)$, $\mathbf{a}_2 = (a/2)(1, \sqrt{3})$ consists of 160×160 atoms. The cell is subjected to the periodic boundary conditions. Discrete breathers are excited in the middle part of the computational cell. In order to absorb the small-amplitude waves emitted by the DB, and ad hoc viscosity term is introduced into the equations of motion for the atoms close to the borders of the computational cell. Horizontal close-packed atomic rows are numbered by the index m, while atoms in the rows by the index n as shown in Figure 1a.

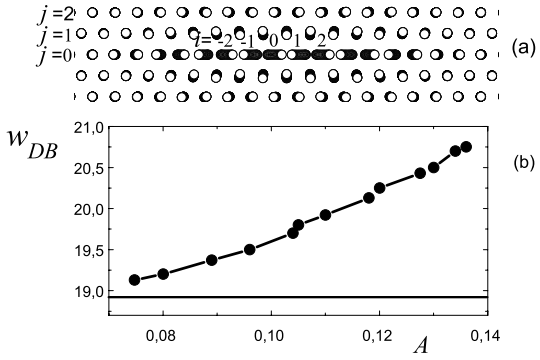

Fig. 1. (a) Stroboscopic picture of atomic motion showing the moving DB excited in the $m = 0$ atomic row with the help of (2), (3) for the parameters $A = 0.128$, $B = 0.015$, $\beta = \gamma = 0.25$, $x_0 = 0$, $\omega = 19.5$, $\varphi_0 = 0.1\pi$, $\delta = 0.04\pi$. (b) DB frequency as the function of amplitude. The upper edge of the phonon band is shown by the horizontal line.

To excite a moving DB in a close-packed row of atoms the following ansatz [64] is used

$$x_n(t) = \cos[\omega t + \varphi_0 + \delta n]X_n^0, \quad y_n(0) = 0, \quad \dot{y}_n(0) = 0, \qquad (2)$$

where ω is the DB frequency, φ_0 is the initial phase, δ is the parameter indicating the phase difference for neighboring atoms, X_n^0 are defined as follows

$$X_n^0 = (-1)^n T_n^0 + S_n^0, \qquad (3)$$

with

$$T_n^0 = \frac{A}{\cosh[\beta(n - x_0)]}, \quad S_n^0 = \frac{-B(n - x_0)}{\cosh[\gamma(n - x_0)]}, \qquad (4)$$

where A is the DB amplitude, B defines the amplitude of displacements of the vibration centers of the atoms, β and γ define the degree of spatial localization of DB, x_0 is the DB initial position. For $x_0 = 0$ the DB is centered on a lattice site, while for $x_0 = 1/2$ midway between two neighboring lattice sites. Thus the functions T_n^0 and S_n^0 in equation (4) describe the amplitudes and the displacements of the vibration centers of the atoms at $t = 0$, respectively. These quantities will be calculated for each period of DB oscillation as

$$T_n = \frac{x_{n,\max} - x_{n,\min}}{2}, \quad S_n = \frac{x_{n,\max} + x_{n,\min}}{2}, \qquad (5)$$

where $x_{n,\max}$ and $x_{n,\min}$ are the maximal and minimal values of the (quasi)periodic function $x_n(t)$ that describes

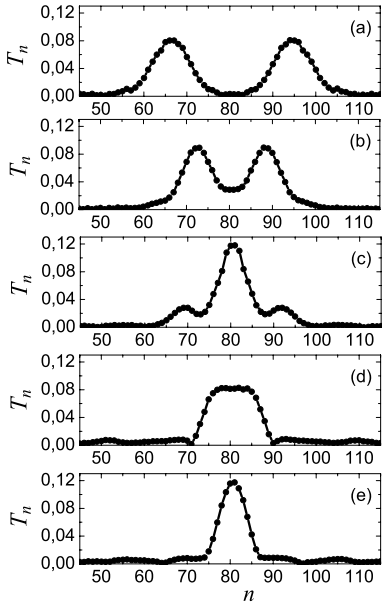

Fig. 2. Head-on collision of DB moving in $m = 0$ atomic row. Panels from the top to the bottom are presented with the time step of 10 time units. As a result of the collision the two DB merge into one having the amplitude larger than the initial DB.

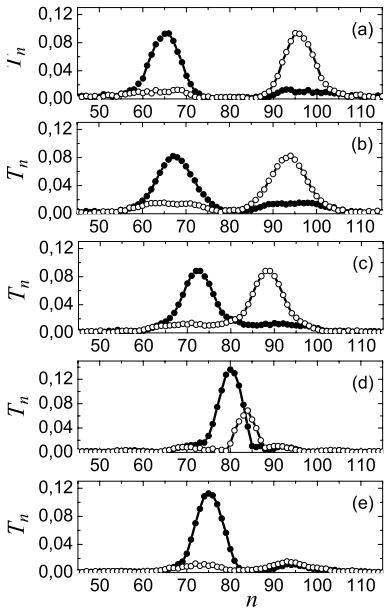

Fig. 3. Head-off collision of DB moving in $m = 0$ (filled dots) and $m = 1$ (open dots) atomic rows. Panels from the top to the bottom are presented with the time step of 10 time units. As a result of the collision the right DB disappears giving a part of its energy to the left DB. The remaining DB moves in the direction opposite to the initial.

the motion of nth atom of a close-packed atomic row. For atoms in the atomic rows where DB is not excited we set $x_n(0) = y_n(0) = 0$ and $\dot{x}_n(0) = \dot{y}_n(0) = 0$. The DB velocity depends on δ, and for $\delta = 0$ it is equal to zero.

It should be noted that the ansatz (2)–(4) is not an exact solution to the equations of motion for the considered 2D crystal. That is why part of the energy given to the system at $t = 0$ is radiated in the form of small-amplitude extended waves and then a stable and robust moving DB emerges, if the parameters in (2)–(4) are properly chosen. Even tough the ansatz (2)–(4) is time periodic, the DB is, generally, speaking not exactly time periodic thus in our study we deal with quasi-DB [55].

In Figure 1a the moving DB excited in the $m = 0$ atomic row is depicted by the stroboscopic picture of atomic motion. The DB is shown at $t = 10$. The following parameter values were used for setting the initial conditions $A = 0.128$, $B = 0.015$, $\beta = \gamma = 0.25$, $x_0 = 0$, $\omega = 19.5$, $\varphi_0 = 0.1\pi$, $\delta = 0.04\pi$. The frequency used to excite the DB is above the phonon spectrum of the crystal. As it can be seen in Figure 1b, the DB frequency, ω_{DB}, increases with the increase in the DB amplitude A. The upper edge of the phonon band, $\omega_{\max} = 18.9$, is shown in (b) by the horizontal line.

3 Interaction of discrete breathers

Here we shall consider a few illustrative cases of head-on and head-off collisions of two identical DB moving toward each other with equal velocities along the x axis (Fig. 1a). For the head-on collision the two DB move in the same atomic row, while for the head-off collisions they move along parallel atomic rows. The initial velocity of DB for the chosen parameter values is $0.35a$ in one time unit.

Figure 2 shows the outcome of a head-on collision where two DB merge forming a single DB with amplitude greater than the initial DB.

For the head-off collisions, the DB moving from the left to the right is always excited in the row $m = 0$ and the DB moving in the opposite direction in a row with $m = 1, 2, \ldots$ The cases $m = 1, 2, \ldots, 10$ and $m = 15$ have been considered. The result of collision depends on m in a non-trivial way. For $m = 1$ and $m = 3$ the scenario presented in Figure 3 is observed. Here one of the breathers decays significantly after the collision thus giving most of its energy and momentum to the other DB. Recall that initially they are identical. Eventually, the dominating surviving DB grows higher in amplitude than its initial value and it moves in the direction opposite to the initial one. For all other values of m, except for $m = 15$, the colliding DB bounce off each other almost elastically. An example for the case $m = 2$ is given in Figure 4. The degree of elasticity of the collision increases with increase in m. For $m = 15$ the DB pass by each other.

4 Conclusions

Several illustrative cases of head-on and head-off collisions of DB in a 2D crystal lattice with intersite Morse potentials were analyzed. For our first approach here only DB that are identical mirror images of each other, moving in the opposite directions with equal velocities have been considered. It was found that the collisions either result in formation of a single DB with amplitude greater than the initial amplitude of the incoming two ($m = 0, 1, 3$) or in

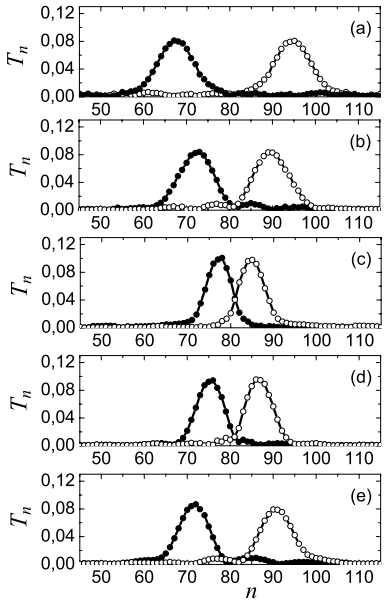

Fig. 4. Head-off collision of DB moving in $m = 0$ (filled dots) and $m = 2$ (open dots) atomic rows. Panels from the top to the bottom are presented with the time step of 10 time units. As a result of the collision the DB bounce off each other almost elastically.

an elastic interaction of DB (other values of m). The elastic interaction is either bounce-off or crossing each other of the two DB. Clearly a mechanism of energy gain by DB becomes available since two colliding DB can produce a DB with the amplitude greater than the initial amplitudes of the colliding DB. This is important because the concept of DB is used to explain various effects observed in crystalline solids [65–69].

The bounce-off was observed for DB moving in the atomic rows $m = \{2, 4, \ldots, 10\}$. It may look strange that DB interact even in the case when they move in well separated rows and with mere intersite potentials. It can be speculated that such a long-range interaction of DB is due to the elastic distortion of the crystal lattice produced by the DB.

The 2D crystal model addressed in this study does not include on-site potential. However, as it can be seen from Figure 1a, as a DB moves along a particular close-packed atomic row the rest of the 2D crystal creates an effective on-site potential. Atoms are not allowed to vibrate with large amplitudes and hence only the repulsive, hard component of the Morse potential operates. This justifies similarities and differences with the genuine (quasi 2D) soliton collisions studied in references [58–63]. We hope that our results are useful to experimenters in their search for applications.

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