

Supplemental Material: A symmetric potential lattice and smooth propagation of tail-free discrete breathers

Yusuke Doi

*Department of Adaptive Machine Systems, Graduate School of Engineering,
Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan*

Kazuyuki Yoshimura

*NTT Communication Science Laboratories, NTT Corporation
3-1 Morinosato, Wakamiya, Atsugi, Kanagawa 243-0198, Japan*

A. DECOMPOSITION OF POTENTIAL IN GENERAL LATTICES

We illustrate the decomposition of potential in detail, using Eq. (9) as an example. Consider the potential (9)

$$\Phi(\mathbf{q}) = \sum_{n=1}^N \left[\frac{1}{2} (q_{n+1} - q_n)^2 + \frac{\alpha}{2} q_n^2 + \frac{\beta}{4} q_n^4 \right] + \sum_{r=1}^{N/2} \sum_{n=1}^N \frac{b_r}{4} (q_{n+r} - q_n)^4, \quad (\text{S1})$$

where α , and β are constants. In the normal mode coordinates, this potential is rewritten as

$$\begin{aligned} \Phi(\mathbf{U}, U_{N/2}) &= 2 \sum_{i=-N_h}^{N_h} U_i U_{-i} \cos^2 \theta_i + \frac{\alpha}{2} \sum_{i=-N_h}^{N_h+1} U_i U_{-i} + \frac{\beta}{4N} \sum_{\substack{i,j,k,l=-N_h \\ i+j+k+l=0, \pm N, 2N}}^{N_h+1} U_i U_j U_k U_l \\ &+ \frac{4}{N} \sum_{\substack{i,j,k,l=-N_h \\ i+j+k+l=0, 2N}}^{N_h+1} \sum_{q=1}^{N/4} [b_{2q-1} c_{(2q-1)i} c_{(2q-1)j} c_{(2q-1)k} c_{(2q-1)l}] U_i U_j U_k U_l \\ &- \frac{4}{N} \sum_{\substack{i,j,k,l=-N_h \\ i+j+k+l=\pm N}}^{N_h+1} \sum_{q=1}^{N/4} [b_{2q-1} c_{(2q-1)i} c_{(2q-1)j} c_{(2q-1)k} c_{(2q-1)l}] U_i U_j U_k U_l \\ &+ \frac{4}{N} \sum_{\substack{i,j,k,l=-N_h \\ i+j+k+l=0, \pm N, 2N}}^{N_h+1} \sum_{q=1}^{N/4} [b_{2q} s_{2qi} s_{2qj} s_{2qk} s_{2ql}] U_i U_j U_k U_l, \end{aligned} \quad (\text{S2})$$

where $\theta_i = 2\pi i/N$ and $c_\alpha = \cos(\alpha\pi/N)$ and $s_\alpha = \sin(\alpha\pi/N)$, respectively. If we decompose the above potential according to the procedure described in the main text, we obtain

$$\begin{aligned} \Phi_s(\mathbf{U}, 0) &= 2 \sum_{i=-N_h}^{N_h} U_i U_{-i} \cos^2 \theta_i + \frac{\alpha}{2} \sum_{i=-N_h}^{N_h} U_i U_{-i} + \frac{\beta}{4N} \sum_{\substack{i,j,k,l=-N_h \\ i+j+k+l=0}}^{N_h} U_i U_j U_k U_l \\ &+ \frac{4}{N} \sum_{\substack{i,j,k,l=-N_h \\ i+j+k+l=0}}^{N_h} \phi^{(i,j,k,l)}(\mathbf{b}) U_i U_j U_k U_l, \end{aligned} \quad (\text{S3})$$

$$\Phi_a(\mathbf{U}, 0) = \frac{\beta}{4N} \sum_{\substack{i,j,k,l=-N_h \\ i+j+k+l=\pm N}}^{N_h} U_i U_j U_k U_l - \frac{4}{N} \sum_{\substack{i,j,k,l=-N_h \\ i+j+k+l=\pm N}}^{N_h} \psi^{(i,j,k,l)}(\mathbf{b}) U_i U_j U_k U_l, \quad (\text{S4})$$

$$\mathcal{R}(\mathbf{U}, U_{N/2}) = \frac{\alpha}{2} U_{N/2}^2 + \frac{\beta}{4N} \left[U_{N/2}^4 + U_{N/2}^2 \sum_{i=-N_h}^{N_h} U_i U_{-i} + U_{N/2} \sum_{\substack{i,j,k=-N_h \\ i+j+k=\pm N/2}}^{N_h} U_i U_j U_k \right]. \quad (\text{S5})$$

Each of the coefficients $\phi^{(i,j,k,l)}(\mathbf{b})$ and $\psi^{(i,j,k,l)}(\mathbf{b})$ is given by a linear combination of the components of $\mathbf{b} = (b_1, b_2, \dots, b_{N/2})$ as follows:

$$\begin{aligned}\phi^{(i,j,k,l)}(\mathbf{b}) &= \sum_{q=1}^{N/4} [b_{2q-1} c_{(2q-1)i} c_{(2q-1)j} c_{(2q-1)k} c_{(2q-1)l} + b_{2q} s_{2qi} s_{2qj} s_{2qk} s_{2ql}], \\ \psi^{(i,j,k,l)}(\mathbf{b}) &= \sum_{q=1}^{N/4} [b_{2q-1} c_{(2q-1)i} c_{(2q-1)j} c_{(2q-1)k} c_{(2q-1)l} - b_{2q} s_{2qi} s_{2qj} s_{2qk} s_{2ql}].\end{aligned}\quad (\text{S6})$$

B. PROPAGATION OF TRAVELING DB IN TRUNCATED PISL

The truncated PISL is constructed by considering only the interactions up to M -th ($M \ll N/2$) nearest neighbor particles and neglecting the other longer-range interactions in Eq. (9). The potential is given by

$$\Phi_M = \frac{1}{2} \sum_{n=1}^N [(q_{n+1} - q_n)^2] + \sum_{r=1}^M \sum_{n=1}^N \frac{b_r}{4} (q_{n+r} - q_n)^4, \quad (\text{S7})$$

where we assumed the case of no on-site potential ($\alpha = \beta = 0$) for comparison with Fig. 7.

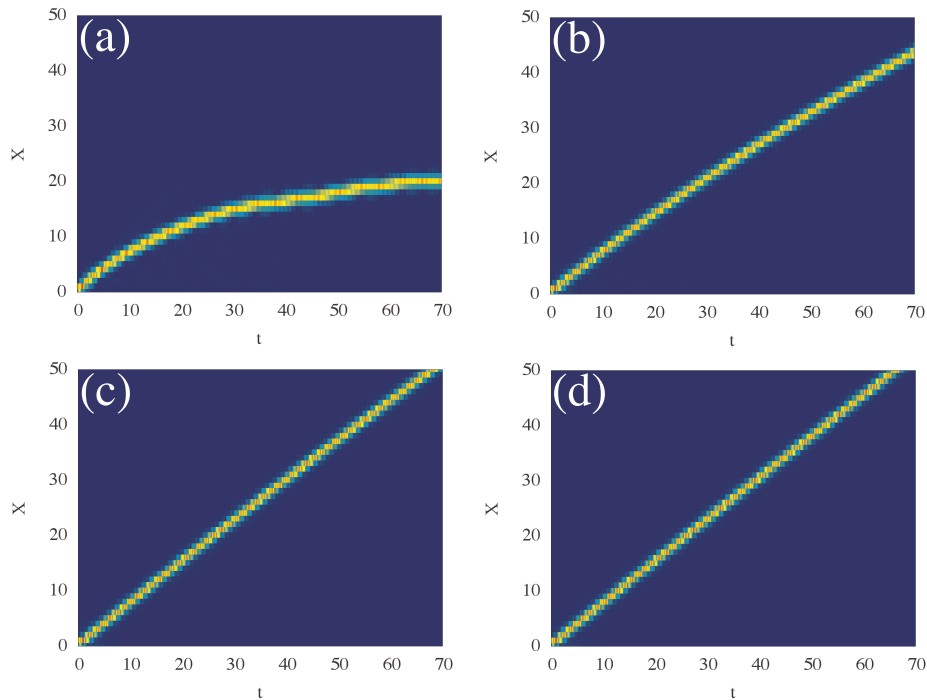


FIG. S1: The center X of traveling DB vs. t in truncated PISL with (a) $M = 1$, (b) $M = 3$, (c) $M = 5$ and (d) $M = 10$.

Figure S1 shows spatio-temporal plots of the site energy of approximate traveling DBs. In Fig. S1(a), the approximate traveling DB in the FPU ($M = 1$) lattice loses its velocity. In Fig. S1(b), velocity loss of the traveling DB becomes smaller, where the long range interactions are retained up to the third nearest neighbor particles. In Fig. S1(c) and (d), the approximate traveling DB recovers an almost constant velocity although the long range interactions only up to $M \ll N/2$ is considered.