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A regularized model equation for discrete breathers in anharmonic lattices with symmetric nearest-neighbor potentials

Bao-Feng Feng[a,*], Yusuke Doi[b], Takuji Kawahara[c]

[a] Department of Mathematics, The University of Texas-Pan American, Edinburg, TX 78541-2999, USA
[b] Department of Adaptive Machine Systems, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan
[c] Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan

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Abstract

We propose a regularized continuum model equation for describing discrete breathers or intrinsic localized modes in one-dimensional anharmonic lattices with symmetric nearest-neighbor potentials. Exact stationary breather solutions with purely hard quartic anharmonicity, as well as approximate stationary breather solutions in the general case, are found. The application of the multiple scales analysis indicates the movability of the small-amplitude breather solutions. The results of numerical simulations for the model equation fully support the analytical solutions. As regards the breather–breather collisions, the continuum model shares many common features with its discrete counterpart, which provides an opportunity to clarify the energy exchange mechanism for collisions between discrete breathers in lattices.

Keywords: Regularized continuum model; Padé approximation; Fermi–Pasta–Ulam lattice; Discrete breather; Intrinsic localized mode; Movability; Multiple scales method; Breather–breather collision

1. Introduction

Since the discovery of intrinsic localized modes (ILMs) or discrete breathers (DBs) in Fermi–Pasta–Ulam (FPU) lattices in the late 1980s [1,2], they have been a topic of increasing focus in view of their significant role in energy localization and transport. DBs are stable time-periodic, highly spatially localized nonlinear modes in discrete lattices, which have been recently observed experimentally in various physical contexts such as coupled optical waveguides [3], Josephson junction ladders [4], antiferromagnet crystals [5], and micromechanical oscillator arrays [6]. A rapidly increasing number of theoretical and numerical studies have been piled up in order to clarify the fundamental properties of ILMs/DBs (see, e.g., the review papers [7–9] and the references therein).

The discreteness of space is a crucial factor for the stability of intrinsic localized modes. The importance of treating the discreteness directly has been recognized and emphasized in the study of intrinsic localized modes. However, it is usually difficult to carry out a general analysis for a nonlinear discrete system, whereas a quasi-continuum approximation can provide an opportunity to understand many general features of the discrete system, because the resulting partial differential equation is more amenable to some analytical and numerical studies.

As a matter of fact, many efforts have been made in this respect [10–12], for which Rosenau developed a systematic methodology for providing continuum approaches to discreteness that makes the present work possible. However, it should be pointed out that several model equations obtained by Rosenau [10] are better approximations to acoustic waves of long wavelength than to optical waves of short wavelength. It is known that intrinsic localized modes belong to optical-like wave excitations. Therefore, it is understandable that these models are inappropriate for describing intrinsic localized modes. On the other hand, Kosevich, by a direct Taylor expansion around the Brillouin-zone edge, derived an envelope-function equation for the optical wave excitations in a discrete

* Corresponding author. Tel.: +1 956 381 2269; fax: +1 956 385 5091.
E-mail address: feng@panam.edu (B.-F. Feng).

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lattice [11]. However, due to the lack of regularity, the resulting model equation is ill-posed and numerically unstable. Furthermore, as far as we are aware, no breather-like solutions have been found based on Kosevich's model.

In the present paper, we propose a regularized model for describing DBs in one-dimensional anharmonic lattices with symmetric nearest-neighbor potentials. As discussed in detail in a subsequent section, we derive our regularized model by applying the so-called staggering transformation firstly to the relative displacement so that the linear spectrum is shifted to the edge of the Brillouin zone, and then the Padé approximation is applied for the envelope of DBs. Thus the quasi-continuum approximation is applied for the envelope such that the spatial variable of the regularized equation has a slow scale different from the original lattice scale. It is shown that the regularized model has two conservation laws, and admits stationary breather solutions in the Fermi–Pasta–Ulam-β atomic lattices. Moreover, a moving breather solution in the small-amplitude limit is obtained by means of the multiple scales method, which can be viewed as an explanation for the movability of intrinsic localized modes in anharmonic lattices. The results of numerical simulations for breather–breather collisions show that they can survive from the collision in most of the cases and share many features with its discrete counterpart. As a result, the approach in the present paper sheds some light on the clarification of some open problems, such as the predictions of the moving DBs and the fundamental features of collisions between DBs from further analysis of the regularized model. On the other hand, it should be pointed out that some inherent features of the discrete system, such as the Peierls–Nabarro (PN) barrier [13] and the periodicity in the dispersion relation, are lost in the process of discrete–continuum transition.

The paper is organized as follows. In Section 2, a regularized model equation for one-dimensional anharmonic lattices with symmetric nearest-neighbor interaction potentials is derived. In Section 3, stationary and moving breather solutions are found by means of a rotating wave approximation (RWA) and a multiple scales method, respectively. Section 4 is devoted to the various numerical simulations for the regularized model for the purpose of verifying the validity of the model and exploring the breather–breather collision properties. The numerical results of the continuum model not only confirm the analytical results in many respects, but also agree with the numerical results for the discrete breathers and the collision properties of two DBs in the FPU-β lattice. The paper is concluded by a discussion.

2. Regularized model equation

We start with a one-dimensional monatomic chain interacting via a nearest-neighbor potential. The Hamiltonian is given by

$$H = \sum_n \left[\frac{1}{2}\dot{y}_n^2 + \Phi(y_{n+1} - y_n) \right], \tag{1}$$

where y_n is the displacement of the n-th particle from its equilibrium position. Φ is the interaction potential between adjacent particles possessing the symmetric property $\Phi(-u) = \Phi(u)$. It is noted here that both the temporal and spatial variables are normalized by the mass and the spacing of particles ($t \to t/\sqrt{m}$, $y_n \to y_n/h$) such that they can be scaled to unit one.

From Eq. (1), the equations of motion turn out to be of the form

$$\ddot{y}_n = T(y_{n+1} - y_n) - T(y_n - y_{n-1}), \tag{2}$$

or can be expressed, in terms of the relative displacement $r_n = y_n - y_{n-1}$, by

$$\ddot{r}_n = T(r_{n+1}) - 2T(r_n) + T(r_{n-1}). \tag{3}$$

Here $T(u) \equiv \partial_u \Phi(u)$ is, obviously, an odd function.

As the discrete breathers are short-wavelength excitations of the chain with wavenumber $\kappa \sim \pi/h$ (h is the lattice spacing, scaled to 1), i.e., near the edge of the Brillouin zone, it is convenient to introduce the so-called staggering transformation: $u(n) = (-1)^n r(n)$, through which Eq. (3) becomes

$$\ddot{u}_n + T(u_{n+1}) + 2T(u_n) + T(u_{n-1}) = 0. \tag{4}$$

As a matter of fact, the staggering transformation implies a shift of π/h is for the spatial wavenumber so that $u(n)$ can be assumed to be slowly varying on the interatomic scale for the optical-like vibration. Thus, $u(n)$ becomes appropriate for the quasi-continuum approximation. Denoting the derivative with respect to the spatial variable x by D_x, using the fact $u_{n\pm1} = \exp(\pm D_x)u(x) = u(x) \pm D_x u + \frac{1}{2}D_x^2 u + \cdots$, we can introduce the following approximation:

$$T(u_{n+1}) + 2T(u_n) + T(u_{n-1}) \approx (4 + D_x^2)T(u) \approx \frac{4T(u)}{1 - D_x^2/4}. \tag{5}$$

Here, the Padé approximation is used as suggested by Rosenau [10]. By means of (5), discrete system (4) is converted into a partial differential equation (PDE) as follows:

$$u_{tt} - \frac{1}{4}u_{xxtt} + 4T(u) = 0. \tag{6}$$

We call Eq. (6) a regularized model equation for the discrete breathers, because we apply a regularizing technique to derive (6), similar to the one used in obtaining the improved Boussinesq equation and the regularized long wave (RLW) equation [14].

Eq. (6) is derivable from the Lagrangian density

$$\mathcal{L} = \frac{1}{2}u_t^2 + \frac{1}{8}u_{xt}^2 - 4\Phi(u). \tag{7}$$

Multiplying Eq. (6) by u_t and u_x respectively, and integrating by parts yields two conservation laws:

$$\int \left(\frac{1}{2}u_t^2 + \frac{1}{8}u_{xt}^2 + 4\Phi(u) \right) \mathrm{d}x = E, \tag{8}$$

$$\int u_x \left(u_t - \frac{1}{4}u_{xxt} \right) \mathrm{d}x = P. \tag{9}$$

Here we call the above two conserved quantities the energy, E, and the momentum, P, respectively. The corresponding energy