The effect of cubic potentials on discrete breathers in a mixed Klein–Gordon/Fermi–Pasta–Ulam chain*

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Nonlinearity has a crucial impact on the symmetry properties of dynamical systems. This paper studies a one-dimensional mixed Klein–Gordon/Fermi–Pasta–Ulam diatomic chain using the expanded rotating plane-wave approximation and numerical calculations to determine the effect of cubic potentials on the symmetry properties of discrete breathers in this system. The results will be very useful to researchers in the field of numerical calculations on discrete breathers.

Keywords: one-dimensional mixed Klein–Gordon/Fermi–Pasta–Ulam diatomic chain, discrete breathers, expanded rotating plane wave approximation, symmetry

PACC: 6320R, 6320P

1. Introduction

Discrete breathers (DBs)[1,2] or intrinsic localized modes are nonlinear collective excitations which play a very important role in condensed matter physics and even in biology. Investigations on DBs have intensified recently due to their experimental generation and observation in chemical compounds,[3] antiferromagnets,[4] coupled arrays of Josephson junctions,[5] Bose–Einstein condensates loaded on optical lattices,[6,7] and myoglobin.[8] The existence of DBs can affect the physical properties of a system, especially the thermodynamical behaviour.[9] Therefore, it is necessary to study the fundamental properties of DBs with more sophisticated spatial symmetries and structures, which will be helpful in understanding their importance for physical applications.

There are many different mathematical methods[10] for finding intrinsic localized modes (DBs) corresponding to different systems. Generally, scientists only consider weak nonlinear potentials; thus localized modes cannot exist far from extended modes in the corresponding linear system. Therefore, reasonable approximations and reductions are used to obtain obvious analytical or numerical solutions from complicated discrete nonlinear equations of motion. Considerable difficulties are encountered in the mathematical technique due to cubic potentials, which is common in real physical systems. The Newton method,[11] commonly adopted for accurate numerical calculation of DBs, is effectively used to overcome these difficulties. However, the effect of cubic potentials on solutions is still not clear, especially with regard to symmetry properties.

In the present paper, we focus on a one-dimensional mixed Klein–Gordon/Fermi–Pasta–Ulam (KG/FPU) diatomic chain.[12] The expanded rotating plane-wave approximation (ERWA)[13,14] is used to investigate the effect of cubic potentials on the symmetry properties of DBs in the mixed KG/FPU chain.

2. The model and ERWA

The general form of the Hamiltonian for a one-dimensional mixed KG/FPU diatomic chain with periodically distributed atoms of alternating masses m and M $(M > m)$ can be written as follows:

$$H = \sum_{i=1}^{N} \left[\frac{1}{2} m_i \dot{u}_i^2 + V(u_i) + W(u_{i+1} - u_i) \right], \quad (1)$$

where m_i is the mass of atom i, the lattice constant $a = 1$, the general on-site potential $V(u)$ for small-amplitude oscillations can be expanded as

$$V(u) = \omega_0^2 \frac{u^2}{2} + \alpha \frac{u^3}{3} + \beta \frac{u^4}{4}, \quad (2)$$

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and the inter-site potential $W(u)$ as

$$W(u) = K_2\frac{u^2}{2} + K_3\frac{u^3}{3} + K_4\frac{u^4}{4}. \quad (3)$$

Thus, the equations of motion take the form

$$\begin{aligned} m_i\ddot{u}_i = & -\left(\omega_0^2 u_i + \alpha u_i^2 + \beta u_i^3\right) \\ & + K_2\left(u_{i+1} + u_{i-1} - 2u_i\right) \\ & + K_3\left[\left(u_{i+1} - u_i\right)^2 - \left(u_i - u_{i-1}\right)^2\right] \\ & + K_4\left[\left(u_{i+1} - u_i\right)^3 + \left(u_{i-1} - u_i\right)^3\right]. \quad (4) \end{aligned}$$

Considering small-amplitude solutions $u_i(t)$ with typical oscillation amplitudes $|u_i| \sim \varepsilon$, they can be formally expanded in a Fourier series as

$$u_i(t) = \sum_{p=-\infty}^{+\infty} a_i^{(p)} \mathrm{e}^{\mathrm{i}\, p\omega_b t}, \quad (5)$$

where ω_b is close to some linear oscillation frequency and the Fourier coefficients $a_i^{(p)}$ depend on time slowly.

According to the ERWA, we reserve the first three terms of Eq. (5) to investigate the static structure of DBs, that is, $\dot{a}_i^{(p)}$ or $\ddot{a}_i^{(p)}$ equals zero. Thus, the trial solution is written as

$$u_i(t) = a_i^{(0)} + a_i^{(1)}\cos(\omega_b t) + a_i^{(2)}\cos(2\omega_b t), \quad (6)$$

where $a_i^{(0)}$, $a_i^{(1)}$ and $a_i^{(2)}$ are called static, first-order harmonic and second-order harmonic coefficients, respectively.

Substituting the solution Eq. (6) into the equations of motion Eq. (4) and reorganizing them to keep the form consistent with Eq. (6), we obtain three series of coupled equations for $a_i^{(0)}$, $a_i^{(1)}$ and $a_i^{(2)}$ as follows: the static part

$$\begin{aligned} 0 = & -\omega_0^2 a_i^{(0)} - \alpha\left[\left|a_i^{(0)}\right|^2 + \frac{1}{2}\left(\left|a_i^{(1)}\right|^2 + \left|a_i^{(2)}\right|^2\right)\right] \\ & - \frac{3}{2}\beta\left(a_i^{(0)}\left|a_i^{(1)}\right|^2 + a_i^{(0)}\left|a_i^{(2)}\right|^2 + \frac{2}{3}a_i^{(0)}\left|a_i^{(0)}\right|^2 + \frac{1}{2}a_i^{(2)}\left|a_i^{(1)}\right|^2\right) \\ & + K_3\left\{\left(a_{i+1}^{(0)} - a_i^{(0)}\right)^2 - \left(a_i^{(0)} - a_{i-1}^{(0)}\right)^2 + \frac{1}{2}\left[\left(a_{i+1}^{(1)} - a_i^{(1)}\right)^2 + \left(a_{i+1}^{(2)} - a_i^{(2)}\right)^2\right]\right. \\ & \left. - \frac{1}{2}\left[\left(a_i^{(1)} - a_{i-1}^{(1)}\right)^2 + \left(a_i^{(2)} - a_{i-1}^{(2)}\right)^2\right]\right\} \\ & + K_4\left\{\left(a_{i+1}^{(0)} - a_i^{(0)}\right)^3 + \left(a_{i-1}^{(0)} - a_i^{(0)}\right)^3 + \frac{3}{2}\left(a_{i+1}^{(0)} - a_i^{(0)}\right)\left[\left(a_{i+1}^{(1)} - a_i^{(1)}\right)^2 + \left(a_{i+1}^{(2)} - a_i^{(2)}\right)^2\right]\right. \\ & + \frac{3}{2}\left(a_{i-1}^{(0)} - a_i^{(0)}\right)\left[\left(a_{i-1}^{(1)} - a_i^{(1)}\right)^2 + \left(a_{i-1}^{(2)} - a_i^{(2)}\right)^2\right] \\ & \left. + \frac{3}{4}\left(a_{i+1}^{(1)} - a_i^{(1)}\right)^2\left(a_{i+1}^{(2)} - a_i^{(2)}\right) + \frac{3}{4}\left(a_{i-1}^{(1)} - a_i^{(1)}\right)^2\left(a_{i-1}^{(2)} - a_i^{(2)}\right)\right\}, \quad (7) \end{aligned}$$

the first-order harmonic part

$$\begin{aligned} -\omega_b^2 m_i a_i^{(1)} = & -\omega_0^2 a_i^{(1)} - \alpha a_i^{(1)}\left(2a_i^{(0)} + a_i^{(2)}\right) - \beta\left(3\left|a_i^{(0)}\right|^2 a_i^{(1)} + \frac{3}{4}\left|a_i^{(1)}\right|^2 a_i^{(1)} + 3a_i^{(0)}a_i^{(1)}a_i^{(2)} + \frac{3}{2}a_i^{(1)}\left|a_i^{(2)}\right|^2\right) \\ & + K_2\left(a_{i+1}^{(1)} + a_{i-1}^{(1)} - 2a_i^{(1)}\right) + K_3\left\{\left(a_{i+1}^{(1)} - a_i^{(1)}\right)\left[2\left(a_{i+1}^{(0)} - a_i^{(0)}\right) + \left(a_{i+1}^{(2)} - a_i^{(2)}\right)\right]\right. \\ & \left. - \left(a_i^{(1)} - a_{i-1}^{(1)}\right)\left[2\left(a_i^{(0)} - a_{i-1}^{(0)}\right) + \left(a_i^{(2)} - a_{i-1}^{(2)}\right)\right]\right\} \\ & + K_4\left\{\frac{3}{4}\left[\left(a_{i+1}^{(1)} - a_i^{(1)}\right)^3 + \left(a_{i-1}^{(1)} - a_i^{(1)}\right)^3\right]\right. \\ & + 3\left(a_{i+1}^{(1)} - a_i^{(1)}\right)\left[\left(a_{i+1}^{(0)} - a_i^{(0)}\right)^2 + \left(a_{i+1}^{(0)} - a_i^{(0)}\right)\left(a_{i+1}^{(2)} - a_i^{(2)}\right)\right] \\ & + 3\left(a_{i-1}^{(1)} - a_i^{(1)}\right)\left[\left(a_{i-1}^{(0)} - a_i^{(0)}\right)^2 + \left(a_{i-1}^{(0)} - a_i^{(0)}\right)\left(a_{i-1}^{(2)} - a_i^{(2)}\right)\right] \\ & \left. + \frac{3}{2}\left[\left(a_{i+1}^{(1)} - a_i^{(1)}\right)\left(a_{i+1}^{(2)} - a_i^{(2)}\right)^2 + \left(a_{i-1}^{(1)} - a_i^{(1)}\right)\left(a_{i-1}^{(2)} - a_i^{(2)}\right)^2\right]\right\}, \quad (8) \end{aligned}$$

and the second-order harmonic part

$$\begin{aligned}
-\omega_b^2 m_i a_i^{(1)} = & -\omega_0^2 a_i^{(1)} - \alpha a_i^{(1)} \left(2a_i^{(0)} + a_i^{(2)}\right) \\
& - \beta \left(\frac{3}{2} a_i^{(0)} \left|a_i^{(1)}\right|^2 + 3\left|a_i^{(0)}\right|^2 a_i^{(2)} + \frac{3}{2}\left|a_i^{(1)}\right|^2 a_i^{(2)} + \frac{3}{4}\left|a_i^{(2)}\right|^2 a_i^{(2)}\right) \\
& + K_2\left(a_{i+1}^{(2)} + a_{i-1}^{(2)} - 2a_i^{(2)}\right) + K_3 \left\{\frac{1}{2}\left[\left(a_{i+1}^{(1)} - a_i^{(1)}\right)^2 - \left(a_i^{(1)} - a_{i-1}^{(1)}\right)^2\right]\right. \\
& \left. + \ 2\left[\left(a_{i+1}^{(0)} - a_i^{(0)}\right)\left(a_{i+1}^{(2)} - a_i^{(2)}\right) - \left(a_i^{(0)} - a_{i-1}^{(0)}\right)\left(a_i^{(2)} - a_{i-1}^{(2)}\right)\right]\right\} \\
& + K_4 \left\{\frac{3}{2}\left[\left(a_{i+1}^{(0)} - a_i^{(0)}\right)\left(a_{i+1}^{(1)} - a_i^{(1)}\right)^2 + \left(a_{i-1}^{(0)} - a_i^{(0)}\right)\left(a_{i-1}^{(1)} - a_i^{(1)}\right)^2\right]\right. \\
& + 3\left[\left(a_{i+1}^{(0)} - a_i^{(0)}\right)^2\left(a_{i+1}^{(2)} - a_i^{(2)}\right) + \left(a_{i-1}^{(0)} - a_i^{(0)}\right)^2\left(a_{i-1}^{(2)} - a_i^{(2)}\right)\right] \\
& + \frac{1}{2}\left[\left(a_{i+1}^{(1)} - a_i^{(1)}\right)^2\left(a_{i+1}^{(2)} - a_i^{(2)}\right) + \left(a_{i-1}^{(1)} - a_i^{(1)}\right)^2\left(a_{i-1}^{(2)} - a_i^{(2)}\right)\right] \\
& \left. + \ \frac{3}{4}\left[\left(a_{i+1}^{(2)} - a_i^{(2)}\right)^3 + \left(a_{i-1}^{(2)} - a_i^{(2)}\right)^3\right]\right\}. \qquad (9)
\end{aligned}$$

3. Numerical results

Maniadis *et al.*[15] have discussed gap breathers in a simple diatomic β-FPU chain involving four types of breather symmetries: the breather with symmetric or antisymmetric profile, which is centred either at a light particle or at a heavy particle. Given $M = 1$, $m = 0.5$, $\omega_0 = 1$, $K_2 = 1$, $N = 201$, we also choose four types of initial conditions to determine how cubic nonlinear potentials affect symmetries of DBs. Each of these initial conditions can be called LSI and HSI (when the initial conditions with symmetric profile are centred at a light and a heavy atom, respectively) and LAI and HAI (when the initial conditions with antisymmetric profile are centred at a light and a heavy atom, respectively).

3.1. Linear dispersion relation

By linearizing the equations of motion around the classical ground state, we can obtain the linear dispersion relation ω_q for each plane-wave solution with wave vector q:

$$\omega_{q\pm} = \frac{1}{2Mm}\left[\left(\omega_0^2 + 2K_2\right)(M+m) \pm \sqrt{\left(\omega_0^2 + 2K_2\right)^2 (M-m)^2 + 16MmK_2^2\cos^2 q}\right]. \qquad (10)$$

From Eq. (10), the following values can be obtained at the centre and the boundary of the Brillouin zone:

$$\begin{aligned}
&\omega_1^2 \equiv \omega_{q-}^2 (q=0), \quad \omega_2^2 \equiv \omega_{q-}^2\left(q = \frac{\pi}{2}\right) = \frac{\omega_0^2 + 2K_2}{M}, \\
&\omega_3^2 \equiv \omega_{q+}^2\left(q = \frac{\pi}{2}\right) = \frac{\omega_0^2 + 2K_2}{m}, \quad \omega_4^2 \equiv \omega_{q+}^2 (q=0). \qquad (11)
\end{aligned}$$

In the following numerical calculations, we choose the frequency of DB to be in the gap of linear dispersion relation, $\omega_b^2 = \frac{1}{2}\left(\omega_2^2 + \omega_3^2\right)$, which satisfies the nonresonant condition.[16]

3.2. Effects of cubic inter-site potential

Given $K_3 = 0.5$, $K_4 = \alpha = \beta = 0$, we calculate Eqs. (7)–(9) to show the results in Figs. 1–4 corresponding to the four types of initial conditions, respectively. The static and second-order harmonic terms are induced by the cubic inter-site potential with special symmetries. Consequently, the second-order harmonic terms have odd symmetry, and the first-order harmonic terms always inherit the symmetry properties of the initial conditions. Moreover, the static terms have odd symmetry only under LSI or LAI initial conditions.

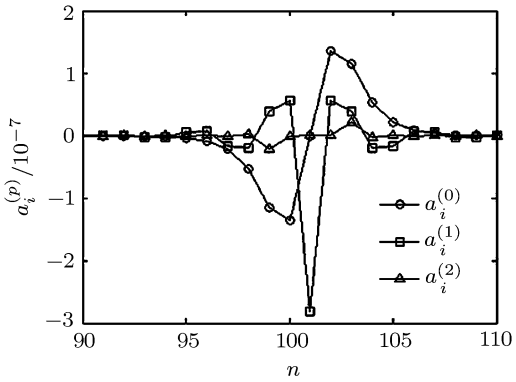


Fig. 1. The profile of the first three Fourier coefficients under the LSI initial condition in the mixed KG/FPU diatomic chain with cubic inter-site potential.

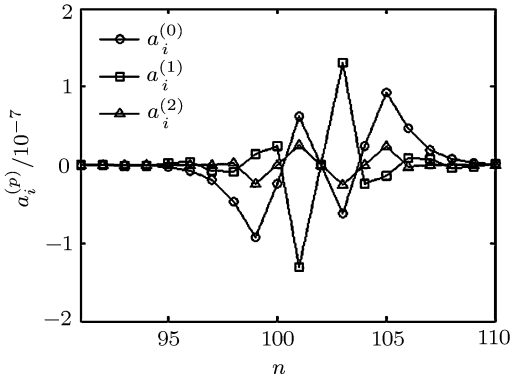


Fig. 2. The profile of the first three Fourier coefficients under the LAI initial condition in the mixed KG/FPU diatomic chain with cubic inter-site potential.

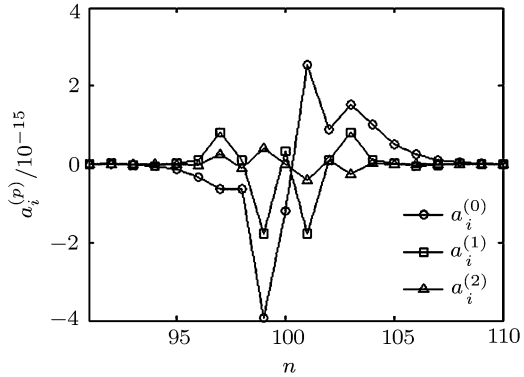


Fig. 3. The profile of the first three Fourier coefficients under the HSI initial condition in the mixed KG/FPU diatomic chain with cubic inter-site potential.

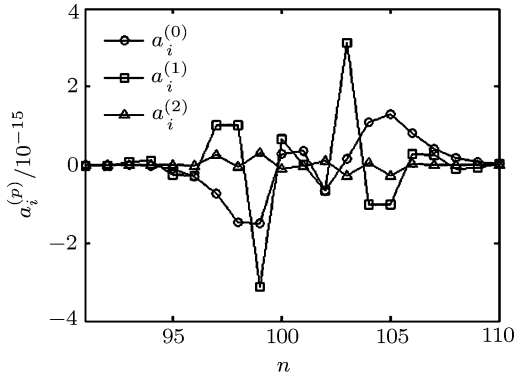


Fig. 4. The profile of the first three Fourier coefficients under the HAI initial condition in the mixed KG/FPU diatomic chain with cubic inter-site potential.

3.3. Effects of cubic on-site potential

Given $\alpha = 0.5$, $K_3 = K_4 = \beta = 0$, we calculate Eqs. (7)–(9) to show the results in Figs. 5–8 corresponding to the four types of initial conditions, respectively. Comparing with the effect of the cubic inter-site potential, the static and second-order harmonic terms can also be induced by the cubic on-site potential, but with even symmetry. Meanwhile, first-order harmonic terms always inherit the symmetries of the corresponding initial conditions.

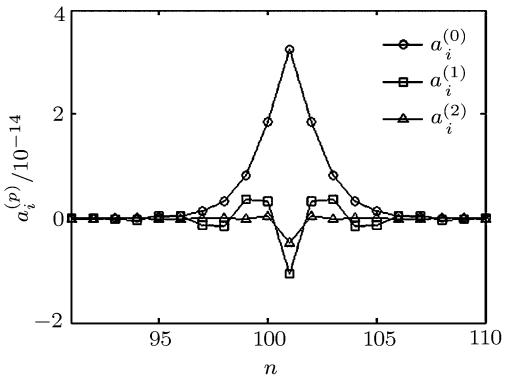


Fig. 5. The profile of the first three Fourier coefficients under the LSI initial condition in the mixed KG/FPU diatomic chain with cubic on-site potential.

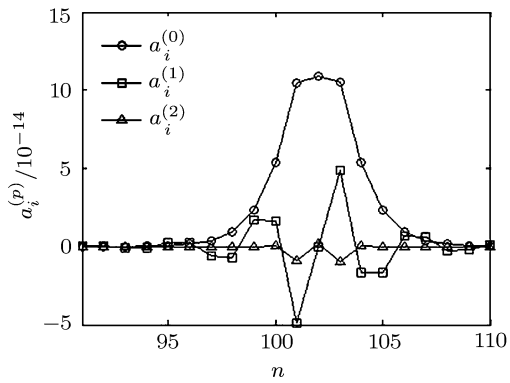


Fig. 6. The profile of the first three Fourier coefficients under the LAI initial condition in the mixed KG/FPU diatomic chain with cubic on-site potential.

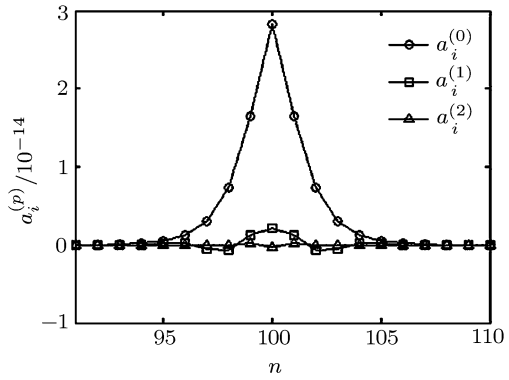


Fig. 7. The profile of the first three Fourier coefficients under the HSI initial condition in the mixed KG/FPU diatomic chain with cubic on-site potential.

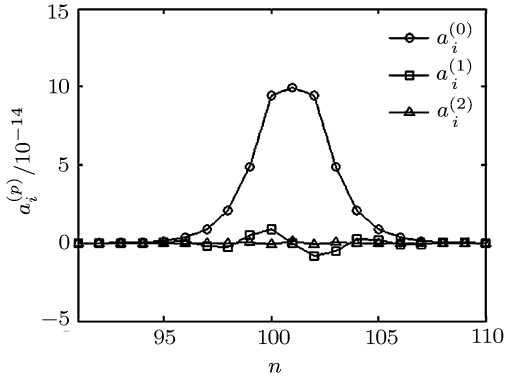


Fig. 8. The profile of the first three Fourier coefficients under the HAI initial condition in the mixed KG/FPU diatomic chain with cubic on-site potential.

4. Conclusions and discussion

The one-dimensional mixed KG/FPU diatomic chain is a complex system, which sustains abundant types of DBs due to bifurcations. It is difficult, and takes considerable time, to obtain significant results systematically by computer. Generally speaking, to grasp the basic essence of the problem is more important and realistic than knowing all the details.

Figures 1–4 show that the cubic inter-site nonlinearity induces static terms with even symmetry under initial conditions of LSI and LAI and second-order harmonic terms with odd symmetry. In contrast, the effect of cubic on-site nonlinearity, shown in Figs. 5–8, is simpler: it induces static terms and second-order harmonic terms with even symmetry under all four initial conditions. In contrast the first-order harmonic terms, as the main oscillation parts, always inherit the symmetries of corresponding initial conditions either with cubic inter- or on-site nonlinear potentials.

As a whole, the two cubic potentials bring about the static and second-order harmonic terms with distinct symmetry. Obviously, the DBs will lose their simple symmetries, as shown in [15], as long as the static or second-order harmonic terms do not possess the same symmetry as the first-order harmonic terms.[17,18] However, there are still some fine symmetries described above. In general, the atomic chain system will sustain DBs with different amplitudes and shapes corresponding to different values of the cubic potentials. Nevertheless, the effect of the cubic potentials on the symmetry of DBs is the same, and so the results obtained above from particular cases have generality.

Nonlinearity has a crucial impact on the symmetry properties of dynamical systems. Consequently the solutions of the dynamical system do not have to come into line with the symmetries of the underlying dynamical system. Fortunately, we can find clear and fine symmetry properties of DBs in the general system through the ERWA, which plays a valuable role in numerical calculations on DBs.

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