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A breather-like localized mode in a Fermi–Pasta–Ulam lattice interacting with an electron

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Abstract. A theoretical study in the framework of a variational approach is presented for the Fermi–Pasta–Ulam (FPU) chain interacting with an extra electron. Standing three-component soliton solutions which describe coupled states of an acoustic polaron with longitudinal lattice vibrations are found. This result is confirmed by numerical simulations and extended qualitatively to a chain with a realistic inter-particle potential of a general form.

1. Introduction

The theory of localized modes appearing on impurities in harmonic lattices with structural disorder is now well developed [1]. In particular, for a one-dimensional lattice with mass impurity these modes are obtained as small-amplitude oscillations (linearized excitations) localized around the mass impurity, so their amplitude decreases exponentially from the impurity centre to infinity. On the other hand, non-linear localized excitations known as intrinsic localized modes [2–5] can exist even in pure but anharmonic lattices (for a review see the recent papers [6, 7]). Further, non-linear localized excitations such as static or moving solitons (topological kinks, polarons etc) with a stationary profile may, to some extent, also be considered as some type of impurity or defect existing in a pure non-linear lattice. Therefore one can expect a localized mode to appear coupled to another coherent structure like a soliton. Recently, localized modes coupled to a discrete topological kink have been studied, and results have been obtained on their spectral properties and creation thresholds [8]. Note that in the continuum limit, the theory of linear modes localized on kinks (domain walls) is now well developed (see the review paper by Jackiw [9]).

Clearly, a similar interest arises in studies of the effects of localization on a non-topological soliton such as a polaron. Vekhter and Ratner [10, 11] have studied numerically the dynamics of electronic localization caused by electron–vibrational interaction. They found a bound electron–breather state. Experimentally, such bound states can be created when incident electrons collide with a thin film [12]. A similar situation also occurs in nanoelectronics, namely, in quantum wells or wires [13]. The discovery of tracks in doped muscovite mica crystals can be understood in terms of breathers interacting with electrons [14, 15]. Recently, Flach and Kladko [16] studied the interaction of a single electron with a discrete breather that can be formed in the Fermi–Pasta–Ulam (FPU) chain. Their problem was formulated as the capture of an electron by a lattice breather without any response of the electron to the breather. Obviously, the presence of an electron interacting with the longitudinal lattice displacement will immediately break the breather symmetry (e.g., in the case of a hard quartic anharmonicity), so a strain (static lattice deformation) component

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occurs in the breather solution. On the other hand, as we shall show in this paper, the appearance of this strain component, i.e., an acoustic polaron, may result in a localization of lattice oscillations even if such a localization effect would be impossible in a pure lattice (without any extra electron). In other words, a single electron can dig a potential well in the lattice not only for itself but also for lattice vibrations, localizing them in a similar manner to the way in which modes are localized on a topological soliton (kink or antikink).

It should also be pointed out that such an effect of self-trapping of the lattice vibrations may happen because the potential well represents a localized contractive deformation of the chain, and hence new equilibria of oscillating chain particles are displaced into the hard repulsive part of the inter-particle potential. Therefore it is expected that the presence of an external electron will result in the appearance of a breather-like localized mode, a mode like that in a pure FPU chain with a hard quartic (symmetric) anharmonicity. This effect is examined in this paper by using a variational approach in the continuum approximation.

2. The model

We consider a chain of particles (atoms, molecules or groups of atoms) of mass M coupled by anharmonic forces (springs) with a characteristic stiffness constant K. The chain particles are constrained to move only along the longitudinal direction and they are supposed to interact with an extra electron. In the adiabatic (semi-classical) limit the Lagrangian function of such a lattice interacting with an electron (or, in general, a quantum quasi-particle) can be written in the form

$$\begin{aligned} L = L\{\dot\psi_n, \psi_n; \dot\psi_n^*, \psi_n^*; \dot Q_n, Q_n\} \\ = \sum_n \Bigg[\mathrm{i}\hbar\psi_n^*\dot\psi_n - E_n\psi_n^*\psi_n + J(\psi_n^*\psi_{n+1} + \psi_{n+1}^*\psi_n) \\ + \frac{1}{2}M\dot Q_n^2 - Mv_0^2 U\left(\frac{Q_{n+1}-Q_n}{l}\right)\Bigg] \end{aligned} \tag{2.1}$$

where the dots denote differentiation with respect to time t. The complex-valued lattice field $\psi_n(t)$ (coefficient functions of the one-electron state vector) describes the probability amplitude of finding the electron at the nth lattice site, so it has to be normalized to unity:

$$\sum_n |\psi_n(t)|^2 = 1. \tag{2.2}$$

The coefficient E_n describes the on-site energy of the electron situated at the nth lattice site and the (positive) constant J is the exchange (overlapping) integral that describes the probability of the electron hopping from site to site (i.e., dispersion in the electron subsystem). The dynamical states of the lattice subsystem are determined by the (real-valued) lattice field $Q_n(t)$, being the displacement of the nth chain particle from its equilibrium position. The (dimensionless) inter-particle potential $U(r)$ is normalized by the relations $U(0) = 0$ and $U''(0) = 1$, so the constant $v_0 = \sqrt{K/M}l$, with l being the lattice spacing, is the characteristic velocity that describes the speed of small-amplitude longitudinal sound along the chain. In general, the potential $U(r)$ can be expanded into a series:

$$U(r) = \sum_{\nu=2}^{\infty} \frac{\kappa_\nu}{\nu} r^\nu. \tag{2.3}$$

For most realistic cases we have $\kappa_j > 0$ if j is even and $\kappa_j < 0$ if j is odd.

In general, the on-site electron energy E_n depends on the distances between the nth particle and its nearest neighbours to the left and right. Expanding this dependence into a power series and keeping only the first-order terms, one can write

$$E_n = E_0 + \chi_L(Q_n - Q_{n-1}) + \chi_R(Q_{n+1} - Q_n) \tag{2.4}$$

where E_0 is the on-site electron energy when the lattice is undistorted, i.e., the chain particles are found in their equilibrium positions, and $\chi_L > 0$ and $\chi_R > 0$ are the constants of the interaction of the electron with the left and the right relative displacements, $Q_n - Q_{n-1}$ and $Q_{n+1} - Q_n$, respectively. In the present paper, we assume that these constants equal each other: $\chi_L = \chi_R = \chi$.

The equations of motion that correspond to the Lagrangian (2.1) with the representation (2.4) are well known (see, e.g., the review paper [17]):

$$\begin{aligned} &\mathrm{i}\hbar\dot{\psi}_n = -J(\psi_{n-1} + \psi_{n+1}) + \chi(Q_{n+1} - Q_{n-1})\psi_n \\ &M\ddot{Q}_n = \frac{Mv_0^2}{l}\left[U'\left(\frac{Q_{n+1} - Q_n}{l}\right) - U'\left(\frac{Q_n - Q_{n-1}}{l}\right)\right] + \chi(|\psi_{n+1}|^2 - |\psi_{n-1}|^2). \end{aligned} \tag{2.5}$$

It is convenient to rewrite these equations in the dimensionless form by using the dimensionless time

$$\tau = \frac{v_0}{l}t \tag{2.6}$$

so that one time unit corresponds to the time interval during of which the (small-amplitude) sound propagates over one lattice spacing period l. We also introduce the dimensionless parameters

$$\alpha = \frac{2\chi l}{J} \qquad \beta = \frac{2\chi l}{Mv_0^2} \qquad \sigma = \frac{Jl}{\hbar v_0} \tag{2.7}$$

and rescale the lattice fields by means of the relations

$$u_n(\tau) = \frac{Q_n(t)}{l} \qquad \phi_n(\tau) = \exp\left(-\frac{2\mathrm{i}J}{\hbar}t\right)\psi_n(t). \tag{2.8}$$

Then the equations of motion (2.5) are transformed into

$$(\mathrm{i}/\sigma)\frac{\mathrm{d}\phi_n}{\mathrm{d}\tau} = -\phi_{n+1} + 2\phi_n - \phi_{n-1} + \frac{\alpha}{2}(u_{n+1} - u_{n-1})\phi_n \tag{2.9}$$

$$\frac{\mathrm{d}^2u_n}{\mathrm{d}\tau^2} = U'(u_{n+1} - u_n) - U'(u_n - u_{n-1}) + \frac{\beta}{2}\left(|\phi_{n+1}|^2 - |\phi_{n-1}|^2\right) \tag{2.10}$$

and the normalization condition (2.2) becomes

$$\sum_n |\phi_n(\tau)|^2 = 1. \tag{2.11}$$

The main goal of the present paper is to describe approximately the breather-like solutions of the equations of motion (2.9) and (2.10) with the constraint (2.11).

3. Truncated equations of motion

We look for a spatially localized and periodic breather-like solution in the lattice and denote it through the function $F_n(\tau)$. On the other hand, the presence of an electron should result in a deformation of the chain which, in its turn, leads to the electron localization. Besides this self-trapping mechanism, a coupling of the electron to a lattice breather or the appearance of a localized oscillating mode in the potential well created by the electron self-trapping

may occur. Therefore, it is reasonable to assume the following *ansatz* for a standing spatial localization:

$$\phi_n(\tau) = \varphi_n \exp(-\mathrm{i}\varepsilon\sigma\tau) \qquad u_n(\tau) = (-1)^n F_n \cos(\Omega\tau) + G_n \tag{3.1}$$

where F_n is a slow-varying (from site to site) amplitude (envelope) of a breather with frequency Ω, G_n is a static part of the chain deformation and ε is the energy of the binding of the electron to the deformation field of the chain. All these variables together with the second (real-valued) envelope φ_n are determined below using different techniques. The first of these is to exclude the time τ by means of the substitution of the *ansatz* (3.1) into the Lagrangian

$$L = \sum_n \left\{ \phi_n^* \left[(\mathrm{i}/\sigma)\frac{\mathrm{d}\phi_n}{\mathrm{d}\tau} + \phi_{n+1} - 2\phi_n + \phi_{n-1} - \frac{\alpha}{2}(u_{n+1} - u_{n-1})\phi_n \right] \right.$$
$$\left. + \frac{\alpha}{\beta}\left[\frac{1}{2}\left(\frac{\mathrm{d}u_n}{\mathrm{d}\tau} \right)^2 - U(u_{n+1} - u_n) \right] \right\} \tag{3.2}$$

which corresponds to the equations of motion (2.9) and (2.10), and then average it over the period 2π. We introduce the static relative displacement field

$$R_n = G_{n+1} - G_n. \tag{3.3}$$

As a result, we get the average Lagrangian $\bar{L}$ which consists of two parts:

$$\bar{L} = \bar{L}_{el} + \bar{L}_{lat}. \tag{3.4}$$

The first part describes the electron subsystem, including its interaction with the lattice. It is given by

$$\bar{L}_{el} = -\sum_n \left[(\varphi_{n+1} - \varphi_n)^2 + \alpha R_n(\varphi_n^2 + \varphi_{n+1}^2)/2 - \varepsilon\varphi_n^2 \right]. \tag{3.5}$$

The second part describes the pure lattice subsystem. Besides the pure breather part, it also contains the coupling of the breather variable F_n with the lattice deformation field R_n. Using the expansion (2.3), by induction we derive the following expression:

$$\bar{L}_{lat} = \frac{\alpha}{\beta}\sum_n \left[\Omega^2 F_n^2/4 - \sum_j (2^j j!)^{-2}(F_n + F_{n+1})^{2j} U^{(2j)}(R_n) \right] \tag{3.6}$$

where the jth derivative of the potential $U(r)$ is denoted by $U^{(j)}(r)$. Here and in what follows the summation over j runs from $j = 0$ to $j = \infty$.

The equations of motion for the fields φ_n, F_n and R_n which follow from the effective Lagrangian (3.4)–(3.6) are

$$\varphi_{n+1} - 2\varphi_n + \varphi_{n-1} - (\alpha/2)(R_{n-1} + R_n)\varphi_n + \varepsilon\varphi_n = 0 \tag{3.7}$$

$$\Omega^2 F_n - \sum_j 4j(2^j j!)^{-2}\left[(F_{n-1} + F_n)^{2j-1} U^{(2j)}(R_{n-1}) + (F_n + F_{n+1})^{2j-1} U^{(2j)}(R_n) \right] = 0 \tag{3.8}$$

$$\sum_j (2^j j!)^{-2}(F_n + F_{n+1})^{2j} U^{(2j+1)}(R_n) + \beta(\varphi_n^2 + \varphi_{n+1}^2)/2 = 0. \tag{3.9}$$

These three equations have to be completed by using the normalization condition

$$\sum_n \varphi_n^2 = 1 \tag{3.10}$$

rewritten in terms of the amplitude φ_n (see equation (2.11)). The discrete equations (3.7) and (3.8) are of Schrödinger type, corresponding to a quantum particle in a potential well.

Thus, the lattice deformation field R_n in equation (3.7) creates a potential well for the electron described by the discrete wave function φ_n. The spectral parameter ε determines the binding energy of the electron–lattice interaction. Equation (3.8) has another spectral parameter, namely Ω^2, and the potential of this Schrödinger-type equation is created by the derivative $U''(R_n)$, including also higher-order derivatives $U^{(2j)}$ with $j \geqslant 2$. Similarly, the breather envelope F_n in equation (3.8) is nothing more than a 'wave function' subject to the potential well formed by the derivatives of $U(R_n)$. Therefore it is reasonable to expect that this potential well can capture the 'quasiparticle' described by the 'wave function' F_n. On the other hand, similarly to the self-trapping effect, equation (3.9) describes the influence of both the φ_n- and the F_n-fields, acting as external forces, on the deformation field R_n. Moreover, one can expect both the electron and the oscillating localized mode with the envelope F_n to dig a potential well for themselves, forming a self-trapped state. Below we will try to analyse such behaviour in the continuum approximation by using a variational approach.

4. The variational approximation

In the continuum approximation the envelopes φ_n and F_n as well as the deformation (strain) field R_n are assumed to vary smoothly from site to site. As a result, the average Lagrange function $\bar{L}$ given by equations (3.4)–(3.6) is transformed to

$$\bar{L} = -\int \left[(\varphi_x^2 + \alpha\varphi^2 R) - \frac{1}{4}(F_x^2 + \Omega^2 F^2) + \sum_j (j!)^{-2} F^{2j} U^{(2j)}(R) \right] \mathrm{d}x. \tag{4.1}$$

The continuum limit of the equations of motion (3.7)–(3.9) can also be obtained immediately from the Lagrangian (4.1):

$$\frac{\delta}{\delta\varphi(x)}\left(\bar{L} + \varepsilon \int \varphi^2(x)\ \mathrm{d}x \right) = \varphi_{xx} - \alpha R\varphi + \varepsilon\varphi = 0 \tag{4.2}$$

$$-\frac{\delta}{\delta F(x)}\bar{L} = F_{xx} - \Omega^2 F + \sum_j 4j(j!)^{-2} F^{2j-1} U^{(2j)}(R) = 0 \tag{4.3}$$

$$-\frac{\delta}{\delta R(x)}\bar{L} = \sum_j (j!)^{-2} F^{2j} U^{(2j+1)}(R) + \beta\varphi^2 = 0. \tag{4.4}$$

In order to analyse these equations qualitatively, we use approximations similar to those suggested by Wattis [18, 19], i.e. the following set of trial functions:

$$\begin{aligned} \varphi(x) &= \sqrt{\frac{\mu}{a(q)}}\,\mathrm{sech}^q(\mu x) \\ F(x) &= F_0\,\mathrm{sech}^p(\mu x) \\ R(x) &= R_0\,\mathrm{sech}^2(\mu x) \end{aligned} \tag{4.5}$$

where the function $a(q)$ is given by the integral

$$a(q) = \int \mathrm{sech}^{2q}(z)\ \mathrm{d}z. \tag{4.6}$$

This trial *ansatz* contains the five variational parameters p, q, μ, F_0 and R_0. This is a minimal number of trial parameters. In general, each of the functions $\varphi(x)$, $F(x)$ and $R(x)$ has its own way of affecting the bell-shaped profile. Therefore, at least three independent parameters should be involved into the variational procedure. In our case it is convenient to have only one parameter (μ) in the arguments of the hyperbolic secant functions and the

two powers p and q which 'correct' the decreasing law of the other two profiles ($\varphi(x)$ and $F(x)$). Besides these parameters which describe the widths of the profiles, we also need the corresponding amplitudes. Since the wave function $\varphi(x)$ is normalized via the equation $\int \varphi^2(x)\,\mathrm{d}x = 1$ which fixes some relation between the width and the amplitude of $\varphi(x)$, the number of the amplitudes is reduced to the two: F_0 and R_0.

Substituting the set of trial functions given by equations (4.5) into the Lagrangian (4.1), we obtain

$$-\bar{L}(p, q, \mu, F_0, R_0) = (\mu^2 q + 2\alpha R_0)\frac{q}{2q+1} - \frac{F_0^2}{4}\left(\frac{p^2\mu}{2p+1} + \frac{\Omega^2}{\mu}\right)a(p) + \mu^{-1}\sum_j (j!)^{-2}F_0^{2j}Z_j \tag{4.7}$$

where

$$Z_j = Z_j(p, R_0) = \int \mathrm{sech}^{2jp}(z)U^{(2j)}[R_0\,\mathrm{sech}^2(z)]\,\mathrm{d}z. \tag{4.8}$$

The Lagrangian (4.7) contains the function $a(p)$ given by the integral representation (4.6). In order to avoid carrying out any operations with this function, we note that the frequency Ω is an arbitrary parameter and the variational parameter p should be somehow related to Ω. If we know such a relation, then the parameter p could be determined uniquely by the frequency Ω. This relation can be found from equation (4.3) in the limit $|x| \to \infty$ when the non-linear terms can be omitted. As a result, the linearized version of equation (4.3) becomes

$$F_{xx} - (\Omega^2 - 4)F = 0 \tag{4.9}$$

and we substitute here the trial function $F(x)$ from equations (4.5). Then the asymptotics of this equation at $|x| \to \infty$ yields the relation

$$\Omega^2 = 4 + p^2\mu^2 \tag{4.10}$$

which can be adopted as a one-to-one correspondence between the parameters Ω and p at each μ to be determined. Therefore we have reduced the total number of the variational parameters to four: q, μ, F_0 and R_0. Since the breather frequency may be considered as a free parameter of the breather solution, we may adopt p in the trial function $F(x)$ (see equations (4.5)) as a free parameter. It is important to note that first we should find extrema of the Lagrangian $\bar{L}(q, \mu, F_0, R_0)$ given by expression (4.7), in which the frequency Ω is considered as a constant. In the equations for extrema we have to substitute Ω^2 according to equation (4.10). Similarly, the $|x| \to \infty$ asymptotics of equation (4.2) gives the binding energy parameter ε:

$$\varepsilon = -q^2\mu^2. \tag{4.11}$$

The equations for determining of the variational parameters q, μ, F_0 and R_0 follow from the extrema conditions $\partial\bar{L}/\partial q = 0$, $\partial\bar{L}/\partial\mu = 0$, $\partial\bar{L}/\partial F_0 = 0$, $\partial\bar{L}/\partial R_0 = 0$. Excluding Ω^2 from these relations by using equation (4.10), we obtain the following set of four equations:

$$q(q+1) = -\alpha R_0/\mu^2 \tag{4.12}$$

$$\mu^2\left[\frac{2q^2}{2q+1}\mu + \frac{p^3 a(p)}{2(2p+1)}F_0^2\right] = \sum_j (j!)^{-2}F_0^{2j}Z_j - a(p)F_0^2 \tag{4.13}$$

$$\sum_j j(j!)^{-2}F_0^{2j-2}Z_j - a(p) = \frac{p^2(p+1)a(p)}{2(2p+1)}\mu^2 \tag{4.14}$$

$$-\sum_j (j!)^{-2} F_0^{2j} Z'_j = 2\beta\mu q/(2q+1) \tag{4.15}$$

where the function $a(p)$ is defined by the integral (4.6) and $Z'_j = Z'_j(p, R_0) = \partial Z_j/\partial R_0$.

The set of equations (4.12)–(4.15) has been written in a form appropriate for an analysis of the existence of solutions. Thus, each of equation (4.12) for determining q and equation (4.13) for determination of μ admit a unique solution because their left-hand sides are monotonically increasing functions of q and μ from zero to infinity, respectively, while their right-hand sides are positive constants (with respect to these parameters). The left-hand sides of the other two equations (4.14) and (4.15) are also monotonically increasing functions in F_0^2 and R_0, respectively, but they are non-zero at $F_0 = 0$ and $R_0 = 0$. More precisely, in equation (4.14), $Z_1 = a(p) + \mathrm{O}(R_0)$, so for sufficiently small amplitudes R_0 this equation is solvable with respect to F_0 and has a unique solution. In equation (4.15) the term with $j = 0$, which does not contain F_0^2, increases from zero because it is $\mathrm{O}(R_0)$ while in each of the terms Z'_j with $j \geqslant 1$ there is a term not involving R_0 but containing F_0^{2j}. Similarly, for sufficiently small F_0^2, equation (4.15) is solvable with respect to R_0. Consequently, the capture of the lattice breather by the electron can occur only if both the amplitudes F_0 and R_0 are sufficiently small. Below we shall examine the existence of such solutions in the examples with cubic and hard quartic anharmonicities.

In order to solve equations (4.12)–(4.15), it is convenient to rewrite equation (4.13) in another form, which does not contain the trial parameter μ. To this end, we substitute μ^2 in the first term of its left-hand side from equation (4.12) while μ^2 in the second term of the left-hand side is substituted for by using equation (4.14). Then, using equation (4.15), we eliminate the terms containing μ. As a result, we obtain

$$\sum_j (j!)^{-2} F_0^{2j} \left[\left(1 - j\frac{p}{p+1}\right) Z_j - \frac{1}{q+1} R_0 Z'_j \right] = \frac{a(p)}{p+1} F_0^2. \tag{4.16}$$

Therefore, equations (4.12), (4.14), (4.15) and (4.16) are basic equations for the determination of the trial parameters q, μ, F_0 and R_0.

5. Polaron and breather limits

It is important to consider the two limiting cases, namely (i) the case where $F_0 \to 0$, which means that only the pure polaron solution is present in the system, and (ii) the case where the electron is absent, for which only the pure FPU breather excitation is considered. For the first case, equation (4.14) is absent and the remaining equations (4.12), (4.15) and (4.16) are solvable. To show this, we note that $Z_j = 0$ for all $j \geqslant 1$ and according to equation (2.3) we have

$$Z_0 = \sum_{\nu=2}^{\infty} \frac{a(\nu)}{\nu} \kappa_\nu R_0^\nu. \tag{5.1}$$

Next, from equation (4.16) one can find that

$$q = R_0 Z'_0/Z_0 - 1 \tag{5.2}$$

and, substituting this value into equation (4.12), we obtain

$$\mu^2 = \alpha Z_0^2/(Z_0 - R_0 Z'_0) Z'_0. \tag{5.3}$$

Now we solve equations (4.15) and (5.3) and find the equation

$$4\alpha\beta^2 Z_0^2 (Z_0 - R_0 Z'_0) = (Z_0 - 2R_0 Z'_0)^2 {Z'_0}^3 \tag{5.4}$$

for the parameter R_0. For any set of the system parameters α and β, equation (5.4) always has a unique solution $R_0 < 0$, and this can be easily concluded if we substitute the series (5.1) in this equation. Having solved equation (5.4), at least numerically, the other variational parameters q and μ are found according to equations (5.2) and (5.3), respectively. In the particular case of the harmonic chain ($\kappa_\nu = 0$ for all $\nu \geqslant 3$), equation (5.4) has the exact solution $R_0 = \alpha\beta^2/8D$ and the other equations (5.2) and (5.3) yield $q = 1$ and $\mu = \alpha\beta/4$. The trial functions $\varphi(x)$ and $R(x)$ in equations (4.5) with these values give the well-known solution representing Davydov's soliton in a molecular chain [17].

Now let us consider the particular case of the potential (2.3) with a hard quartic anharmonicity. For this case all $\kappa_\nu = 0$, except that $\kappa_4 > 0$, and the stable FPU breather mode is known to exist [4]. In order to get this case from the general equations, it is sufficient to put $\nu = 0$, $R_0 = 0$ and $p = 1$ in equations (4.13) and (4.14). Then all $Z_j = 0$, except that $Z_1 = 2$ and $Z_2 = 8\kappa_4$, and both of these equations are reduced to the relation $\mu^2 = 6\kappa_4 F_0^2$. The trial function $F(x)$ in equations (4.5) with this value for μ and $p = 1$ as well as the relation (4.10) give the exact continuum solution of equation (4.3) which agrees with that in [2]. Below we shall also consider two particular cases of cubic and quartic anharmonicities but with the presence of an electron.

6. Cubic and quartic anharmonicities

In the particular case of a cubic anharmonicity the functions Z_j are easily calculated to yield

$$Z_0 = \frac{2}{3}R_0^2\left(1 + \frac{8}{15}\kappa_3 R_0\right) \qquad Z_1 = a(p)\left(1 + \frac{4p}{2p+1}\kappa_3 R_0\right) \tag{6.1}$$

and $Z_j = 0$ for all $j \geqslant 2$. Next, from equation (4.14) we immediately find that

$$\mu^2 = 8\kappa_3 R_0/p(p+1) \tag{6.2}$$

so the amplitude R_0 must be negative. Inserting this value into equation (4.12), we find that the parameter q satisfies a quadratic equation which always has a unique positive root:

$$q = \frac{1}{2}\left(\sqrt{8\lambda_3 + 1} - 1\right) \tag{6.3}$$

with $\lambda_3 = -p(p+1)\alpha/16\kappa_3$. Next, equation (4.16) yields the solution for the amplitude F_0:

$$F_0^2 = \frac{(p+1)(2p+1)}{6pa(p)(q-p)}R_0\left[\frac{1-q}{\kappa_3} + \frac{8}{15}(2-q)R_0\right]. \tag{6.4}$$

Finally, inserting this solution into equation (4.15) and using (6.2), we find that the other amplitude R_0 satisfies the equation

$$\sqrt{2\kappa_3 R_0}\left[\frac{p-1}{2\kappa_3} + \frac{4}{15}(p-2)R_0\right] = \frac{6q(q-p)\beta}{\sqrt{p(p+1)}(q+1)(2q+1)}. \tag{6.5}$$

In the particular case $p = 1$ this equation is simplified to yield the solution

$$R_0 = 3\left[\frac{5(q-1)q\beta}{4(q+1)(2q+1)}\right]^{2/3}\left(\frac{3}{\kappa_3}\right)^{1/3}. \tag{6.6}$$

It follows from the last equations that the parameter q must be in the interval $1 < q < 2$. Therefore, from the solution (6.3), the system parameters are constrained to satisfy the

inequalities $1 < \lambda_3 < 3$. If λ_3 is sufficiently close to 1, then the inequality $\kappa_3 R_0 \ll 1$ holds. On the other hand, in this limit we can find approximately from equation (4.4) that

$$R \simeq -(2\kappa_3 F^2 + \beta\varphi^2) \tag{6.7}$$

and, inserting this expression into equations (4.2) and (4.3), we find

$$\varphi_{xx} + \alpha\beta\varphi^3 + 2\alpha\kappa_3 F^2\varphi + \varepsilon\varphi = 0 \tag{6.8}$$

$$F_{xx} - (\Omega^2 - 4)F - 16\kappa_3^2 F^3 - 8\beta\kappa_3\varphi^2 F = 0. \tag{6.9}$$

The approximate equations (6.8) and (6.9) admit the exact soliton solution in the limit $\lambda_3 \to 1$ (or $q \to 1$) which is defined by the functions (4.5) with μ given by equation (6.2). Instead of the expression (6.6), in this case we have the equation

$$R_0 + \beta\sqrt{\kappa_3 R_0} + 2\kappa_3 F_0^2 = 0 \tag{6.10}$$

with respect to R_0 where F_0 appears to be a free parameter. Equation (6.10) has a solution if F_0 is bounded from above, according to the inequality $F_0 \leqslant \beta/2\sqrt{2}$.

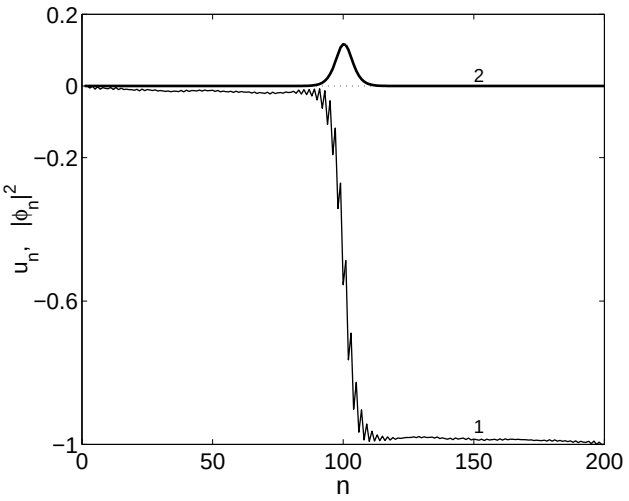

Figure 1. The polaron-breather profile obtained after the integration time $\tau_i = 10\,000 = 3199T$ for the chain with the parameters $\alpha = \beta = 1$, $\sigma = 1$ and $\kappa_3 = -0.125$. Curve 1 represents the lattice displacements $u_n(\tau_i)$ and curve 2 represents the probability distribution $|\phi_n(\tau_i)|^2$ at the final time τ_i.

We have checked the analytical solutions obtained above by numerical tests. We substituted these solutions into the equations of motion (2.9) and (2.10) and integrated them by using the fourth-order Runge–Kutta method with the time step $\Delta\tau = 0.01$ for a chain consisting of $N = 200$ particles. We chose the parameter values $\alpha = \beta = 1$, $\sigma = 1$ (see their definitions (2.7)) and $\kappa_3 = -0.125$. We considered wide solutions, in order to satisfy the continuum approximation. In this case of breather amplitude $F_0 = 0.1$ we have $\mu = 0.19$, so the breather is sufficiently wide. The frequency of the breather is $\Omega = 2.01$ and the oscillation period is, consequently, $T = 2\pi/\Omega = 3.126$. The profile after an integration time $\tau_i = 10\,000 \simeq 3199T$ is shown in figure 1. Here the initial condition for the strain part in equation (3.1) has been used in the conventional kink-shape form (see equations (3.3) and (4.5)): $G(z) = (G_0/\mu)\tanh(\mu z)$. The solid line represents the displacement field u_n while the dashed one describes the probability distribution $|\phi_n|^2$. The form of this localized

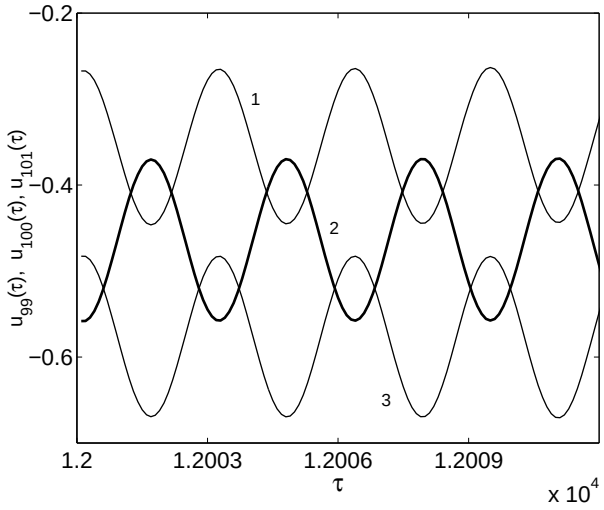

Figure 2. The time dependence $u_n(\tau)$ for three central particles of the polaron-breather profile: $n = 99, 100$ and 101 (curve 1, curve 2 and curve 3, respectively) for the same chain.

solution is essentially unchanged from the initial conditions at $\tau = 0$. The precision of the integration was checked by monitoring the total energy of the system and the normalization condition (2.11). The calculations show the conservation of these quantities up to five digits. The time evolution of the lattice displacements of the three central particles for the numbers $n = 99$ (curve 1), $n = 100$ (curve 2) and $n = 101$ (curve 3) over several oscillation periods is plotted in figure 2. The shape of these dependencies is an additional demonstration that we have obtained a localized periodic solution.

In the case of a narrower breather ($\alpha = \beta = 1.6$, $\sigma = 1$, $\kappa_3 = -0.2$, $F_0 = 0.2$), we observed a similar situation; however, some radiation appears at the edges. Therefore more discrete solutions are not approximated as accurately by our scheme.

The case with a hard quartic anharmonicity is less interesting from the physical point of view. Nevertheless, we also consider this case, because it is popular as a typical example of the existence of intrinsic localized modes [2–7]. For this case we have

$$Z_0 = \frac{2}{3}R_0^2\left(1 + \frac{12}{35}\kappa_4 R_0^2\right) \qquad Z_1 = 2\left(1 + \frac{8}{5}\kappa_4 R_0^2\right) \qquad Z_2 = 8\kappa_4 \tag{6.11}$$

and $Z_j = 0$ for all $j \geqslant 3$. Inserting these values into equations (4.14) and (4.16), we find

$$F_0^2 + 4R_0^2/5 = \mu^2/6\kappa_4 \tag{6.12}$$

$$F_0^2 + R_0^2/7 = 5(q-1)/12(3-q)\kappa_4 \tag{6.13}$$

respectively. Using equation (6.13), from equation (4.15) we get

$$R_0 = -\frac{3(3-q)q}{2(q+1)(2q+1)}\beta\mu. \tag{6.14}$$

Then, using equation (6.14), we find from equation (4.12) the dependence $\mu = \mu(q)$:

$$\mu = \mu(q) = \frac{3(3-q)}{2(q+1)^2(2q+1)}\alpha\beta. \tag{6.15}$$

The equation for determination of the parameter q can be found if we solve equations (6.12) and (6.13) with respect to F_0 and R_0. As a result, we find the equation

$$\frac{23[3(3-q)]^5 q^2}{70(q+1)^2(2q+1)^2}\alpha^2\beta^4\kappa_4 = 9(3-q)^3\alpha^2\beta^2 - 10(q-1)(q+1)^4(2q+1)^2 \tag{6.16}$$

with respect to the parameter q. It can easily be seen from this equation that it admits a unique root if the inequality

$$\beta^2\kappa_4 < 1 \tag{6.17}$$

holds. Having found this parameter, the other parameters μ, F_0 and R_0 are calculated directly according to equations (6.13)–(6.16).

7. Conclusions

In this paper we have investigated the problem of the self-consistent interaction of a single electron with longitudinal lattice vibrations. Due to the complexity of the breather–electron interaction, and in order to simplify the analysis as much as possible, we have restricted ourselves to considering only one (background) harmonic of the breather oscillations. Instead, the problem is studied in a self-consistent way when the electron response to the lattice breather is taken into account. Therefore our results are mainly qualitative and they are valid only for sufficiently wide and low-amplitude oscillations. For such breather-like excitations we have developed a variational procedure for any realistic potential. A set of general equations has been obtained which shows the existence of a small-amplitude wide breather-like excitation in the presence of an electron interacting with the chain. We have obtained a standing small-amplitude breather in the FPU chain with negative cubic anharmonicity on the polaron background while it is well known that such a lattice does not support 'intrinsic' breather solutions because inequality (5.15) of [2] (or inequality (3.34) of [20]) does not hold.

The investigation presented in this paper differs from that of Flach and Kladko [16] in two respects. First, we consider the electron–lattice interaction in a self-consistent way, while in the paper [16] the influence of the electron on the breather dynamics was not taken into account. Second, Flach and Kladko considered highly discrete (localized) breather solutions. Starting from a given breather solution localized at one lattice site, they found the profile for the electron wave function. As a result, capture of an electron has been shown to occur during each half-period of the breather oscillations. We have considered the 'opposite' limit in which the lattice oscillations are sufficiently extended that the continuum approximation can be applied. The presence of an electron in the chain causes a static lattice deformation which creates a potential well, not only for the electron, but also for the lattice vibrations. This localizes the two effects and forms a breather-like state. Note that this coupled state can appear only in the case in which the chain contains an anharmonicity. Moreover, the existence of a pure lattice breather is not a necessary condition for the formation of such coupled breather-like states; the latter can exist even in the case in which pure lattice breathers cannot be created, e.g., in the FPU chain with cubic anharmonicity.

Of course, the variational procedure developed in this paper is rather crude because higher-order lattice-vibration harmonics were not included in the *ansatz* (3.1). Also, the electron probability distribution in this *ansatz* was taken to be averaged in the region of the breather excitation. For narrow breathers we should improve the *ansatz* (3.1), taking into account its 'fine' structure. Finally, the present theory could be extended to the case of moving excitations and Wattis's approximation techniques would be useful for

such investigations. These problems are now being studied and results will be published elsewhere.

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