Discrete Breathers in Systems with Homogeneous Potentials: Analytic Solutions

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We construct lattice Hamiltonians with homogeneous interaction potentials which allow for explicit breather solutions. Especially we obtain exponentially localized solutions for d-dimensional lattices with $d = 2, 3$.

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The understanding of dynamical localization in classical spatially extended and ordered systems [1] experienced recent considerable progress [2–4]. Specifically time-periodic and spatially localized solutions of the classical equations of motion exist, which are called (discrete) breathers, or intrinsic localized modes. The attribute discrete stands for the spatial discreteness of the system, i.e., instead of field equations one typically considers the dynamics of degrees of freedom ordered on a spatial lattice. The lattice Hamiltonians are invariant under discrete translations in space. The discreteness of the system produces a cutoff in the wavelength of extended states, and thus yields a finite upper bound on the spectrum of eigenfrequencies Ω_q (phonon band) of small-amplitude plane waves (one usually assumes that usually for small amplitudes the Hamiltonian is in leading order a quadratic form of the degrees of freedom). If now the equations of motion contain nonlinear terms, the nonlinearity will in general allow one to tune frequencies of periodic orbits outside of the phonon band, and if all multiples of a given frequency are outside the phonon band too, there seems to be no further barrier preventing spatial localization (for reviews, see [2,3]).

Discrete breathers have been recently experimentally detected in weakly coupled waveguides [5], MX solids [6], and Josephson junction ladders [7]. The broad spectrum of applicability of the localization concept described above makes it worthwhile to continue theoretical efforts to characterize the properties of discrete breathers.

So far there is very little knowledge about explicit forms of breather solutions. Except for trivial limiting cases like the anti-integrable limit, i.e., the case of uncoupled degrees of freedom [8], we know only about the solutions of the Ablowitz-Ladik lattice [9] (an integrable one-dimensional variant of the nonlinear Schrödinger equation). What is generically available is the abstract knowledge about existence or nonexistence of discrete breathers for a specific system, and the spatial decay properties far from the center of the breather, where due to the smallness of the amplitudes linearizations or other perturbation techniques are applicable. Note that generically breathers can appear in nonintegrable systems.

From the above it appears that nonintegrability spoils the possibility to obtain analytic forms of the breather solution. We will show that this is not the case by constructing Hamiltonians which allow for explicit solutions and are most probably not integrable. Moreover we will even construct solutions for two- and three-dimensional lattices. Although these models are not motivated by certain applications, the study of their properties can be helpful with respect to discrete breathers.

A bond-ordered quasilinear chain.—In this section we consider a one-dimensional model with the Hamiltonian,

$$H = W_k + W_p, \qquad W_k = \sum_l \frac{1}{2} p_l^2,$$
$$W_p = \frac{1}{2} \sum_l (x_l - x_{l+1})^2 h(s_l), \tag{1}$$
$$s_l(\{x_{l'}\}) = \frac{x_l}{x_{l+1}} + \frac{x_{l+1}}{x_l}.$$

The integer l marks the lattice sites of the chain. The equations of motion read

$$\dot{x}_l = p_l, \qquad \dot{p}_l = -\frac{\partial W_p}{\partial x_l}. \tag{2}$$

Since we are interested in obtaining solutions which decay to zero at spatial infinities and can be interpreted as excitations above some regular ground state $x_l = 0$, we demand that $h(s)$ behaves regularly and especially that $h(s \to \pm\infty)$ does not diverge. The potential energy W_p is a homogeneous function of the coordinates x_l since $W_p(\{\lambda x_l\}) = \lambda^2 W_p(\{x_l\})$. The homogeneity of the potential function can be used to separate time $[G(t)]$ and space (u_l) variables as done, e.g., in [10,11],

$$x_l(t) = u_l G(t), \qquad \ddot{G} = -\kappa G,$$
$$-\kappa u_l = -\frac{\partial W_p(\{u_{l'}\})}{\partial u_l}. \tag{3}$$

Here $\kappa > 0$ is needed to ensure the boundness of the solutions. Indeed the time dependence is then given by

$$G(t) = A\cos(\omega t + \phi), \qquad \omega^2 = \kappa. \tag{4}$$

The equations for the spatial amplitudes u_l read

$$\kappa = \left(1 - \frac{u_{l+1}}{u_l}\right) h(s_l) + \left(1 - \frac{u_{l+1}}{u_l}\right)^2 h'(s_l) p_l + \left(1 - \frac{u_{l-1}}{u_l}\right) h(s_{l-1}) - \left(1 - \frac{u_{l-1}}{u_l}\right)^2 h'(s_{l-1}) p_{l-1}, \tag{5}$$

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$$p_l = \frac{u_l}{u_{l+1}} - \frac{u_{l+1}}{u_l}, \tag{6}$$

and $s_l \equiv s_l(\{u_{l'}\})$. Here $f'(x)$ means the first derivative of f with respect to x. We are looking for a solution of $\{u_{l'}\}$ which is localized in space, i.e., $u_{l\to\pm\infty} \to 0$. In order to find such a solution to (5) we assume that s_l is constant in the spatial tails. This condition is equivalent to having exponential decay. Taking

$$u_l = (-1)^l e^{-\beta|l|} \tag{7}$$

and combining the two different cases $l = 0$ (center of the solutions) and $l \neq 0$ (tails of the solution) we find

$$h(-s) = -s(s+1)h'(-s), \qquad s = 2\cosh(\beta), \tag{8}$$

and

$$\kappa = [2 + s(1-\gamma)]h(-s) \times \left\{1 + \frac{\gamma}{s+1}\gamma\left[1 + \frac{s}{2}(1-\gamma)\right]\right\}, \tag{9}$$
$$\gamma = \sqrt{1 - \left(\frac{2}{s}\right)^2}.$$

Suppose there exists a value for $s = s_0 > 2$ such that (8) is satisfied. If for this value we also have $h(-s) > 0$ then (9) defines a positive value for κ. Moreover the found solution s_0 of (8) will be structurally stable against changes in $h(s)$. Such models can be generated by starting with the trivial case $h(s) = 1$. A strong enough local distortion in $h(s)$ at $s < -2$ will generate solutions of the above equations, preserving the overall positivity and boundness $a > h(s) > 0$ for all s with finite a. Thus the state $x_l = c$ (here c is an arbitrary constant) will be a state with minimum energy $H = 0$, with all other trajectories having larger energies. We can therefore interpret the found explicit localized time-periodic solution (7) as a discrete breather solution, an excitation above a classical homogeneous ground state.

Let us consider an example. Choose

$$h(s) = 1 + ae^{-bs^2}. \tag{10}$$

For parameters

$$a > \frac{e^{3/2}}{2 + 3\sqrt{3/(2b)}}, \qquad b > \frac{3}{8}, \tag{11}$$

there is at least one solution to (8) with $s > 2$. This solution is structurally stable against perturbations in $h(s)$. For example, for $b = 0.5$ and $a = 0.7$ the solution is $s \approx 2.06781$ and $\beta \approx 0.25967$.

Why did we choose a staggered solution $u_l \sim (-1)^l$? This is motivated by the fact that we consider perturbed harmonic chains [$h(s) = 1$] for which the spectrum of plane waves is acoustic. Thus discrete breathers in order to localize should show up with frequencies above the acoustic phonon band which implies out-of-phase motion of nearest neighbors, or simply staggered solutions. It is not that simple to apply these arguments to the case of $h(s) \neq 1$, since there is no simple way to linearize the equations of motion around $x_l = 0$ in the general case. Without going into further details, let us state here that by using a nonstaggered ansatz one arrives at equations which do not ensure positivity of κ in general.

Let us study the problem of small amplitude excitations above the ground state of (1). First we recall that we consider only positive and bounded functions $h(s)$. Then there exists a continuous family of ground states, i.e., solutions with the lowest possible energy $E = 0$ and $\dot{x}_l = 0$ which are given by

$$x_l = c. \tag{12}$$

Notice that the Hamiltonian (1) is not invariant under transformations $x_l \to c + x_l$, yet the ground state energy is degenerate. An expansion around one of the ground states yields

$$W_p = \frac{c^2}{2}\sum_l [h(2)(\delta_l - \delta_{l+1})^2 + h'(2)(\delta_l - \delta_{l+1})^4 + O(\delta^5)], \tag{13}$$
$$\delta_l = \frac{x_l}{c} - 1.$$

The neglected terms of fifth and higher orders in (13) are not invariant under transformations $\delta_l \to \tilde{c} + \delta_l$. However the terms up to fourth order are invariant. Taking into account only terms up to fourth order thus yields a so-called Fermi-Pasta-Ulam chain for the dynamics of small deviations from the ground state $x_l = c$. Note that we cannot simply perform the limit $c \to 0$ since the expansion (13) is valid only if $|\delta_l| \ll c$. The above found breather solution, which decays to zero at infinities (and not to $c \neq 0$), cannot be easily deformed in order to decay to $c \neq 0$ at infinities. However it is well known that (13) allows for discrete breather solutions if $h'(2) > 0$ (which cannot be given in a closed analytical form) (e.g., [12–14]). So we conclude that for the considered model (1) discrete breather excitations above the ground state $x_l = c \neq 0$ are solutions with generic features, and the ground state $x_l = 0$ allows for discrete breather excitations given in a closed analytical form.

In the last part of this section we will discuss the existence of different variants of discrete breathers with $x_{l\to\infty} \to 0$ asymptotics. The existence of the above derived discrete breather solution can be interpreted as follows. Our ansatz $u_l = (-1)^l e^{-\beta|l|}$ contains together with the parameter κ [coming from separating time and space in (3)] two parameters to be determined—β and κ. With our ansatz we found two equations—one for the spatial wings of the solution, and one for the center. Two equations with two variables can be solved in general, and the additional inequality $\kappa > 0$ will serve as an additional restriction for the choice of possible functions $h(s)$, but will not change the fact that once solutions are found, they will be in general structurally stable against changes in $h(s)$. Let us now look for a solution of the form $u_l = e^{-\beta l}$ for

$l \geq 0$; $u_l = ae^{\beta' l}$ for $l \leq -1$. We now have four equations—two in the tails, one at $l = 0$, and one at $l = -1$, and four parameters—κ, β, β', and a. So we conclude that in general such solutions will exist. Indeed, the solution from above is a variant of the more general case discussed here with $a = 1$ and $\beta' = \beta$. So we can expect in general a countable set of other solutions with $a \neq 1$ and $\beta' \neq \beta$. All these solutions will have a closed analytical form with parameters to be determined numerically from the mentioned equations.

Site ordered models in D dimensions.—Consider a d-dimensional hypercube lattice with a scalar coordinate $x_{\mathbf{l}}$ associated to each lattice site. The site index $\mathbf{l} = (l_1, l_2, \ldots, l_d)$ is a d-dimensional vector with integer components l_i. Consider the operator $\hat{L}$ defined as

$$\hat{L} x_{\mathbf{l}} = \sum_{\mathbf{l}', |\mathbf{l}' - \mathbf{l}| = 1} x_{\mathbf{l}'} . \tag{14}$$

Here $|\mathbf{l}|^2 = l_1^2 + l_2^2 + \cdots + l_d^2$. Also define

$$s_{\mathbf{l}} = \frac{\hat{L} x_{\mathbf{l}}}{x_{\mathbf{l}}} . \tag{15}$$

The Hamiltonian is given by a sum over kinetic and potential energies as in (1), with the potential energy

$$W_p = \frac{1}{2} \sum_{\mathbf{l}} (\hat{L} x_{\mathbf{l}})^2 h(s_{\mathbf{l}}) . \tag{16}$$

Assuming time-space separability as in (3) we obtain

$$\ddot{G} = -\kappa G \tag{17}$$

for the time dependence. Again we need $\kappa > 0$ to ensure bounded solutions.

The spatial coordinates have to satisfy an equation similar to (3). Let us calculate the derivative

$$\frac{\partial W_p}{\partial u_{\mathbf{l}}} = \frac{\partial}{\partial u_{\mathbf{l}}} \left[\frac{1}{2} (\hat{L} x_{\mathbf{l}})^2 h(s_{\mathbf{l}}) \right] + \frac{\partial}{\partial u_{\mathbf{l}}} \hat{L} \left[\frac{1}{2} (\hat{L} x_{\mathbf{l}})^2 h(s_{\mathbf{l}}) \right] . \tag{18}$$

Evaluation of these equations leads to the result

$$\kappa u_{\mathbf{l}} = -\frac{1}{2} u_{\mathbf{l}} s_{\mathbf{l}}^3 h'(s_{\mathbf{l}}) + \hat{L}[u_{\mathbf{l}} s_{\mathbf{l}} h(s_{\mathbf{l}})] + \frac{1}{2} \hat{L}[u_{\mathbf{l}} s_{\mathbf{l}}^2 h'(s_{\mathbf{l}})] . \tag{19}$$

A closer study of Eq. (19) shows that it could be easily solved if $s_{\mathbf{l}}$ is essentially constant everywhere on the lattice, more precisely everywhere except for one site $\mathbf{l} = \mathbf{0}$,

$$s_{\mathbf{l} \neq \mathbf{0}} = s_1 , \qquad s_{\mathbf{l} = \mathbf{0}} = s_0 . \tag{20}$$

In that case evaluation of (19) yields

$$\kappa = s_1^2 h(s_1), \qquad |\mathbf{l}| > 1 , \tag{21}$$

$$\kappa = s_1^2 h(s_1) + \frac{u_{\mathbf{0}}}{u_{\mathbf{l}}} \left[s_0 h(s_0) + \frac{1}{2} s_0^2 h'(s_0) - s_1 h(s_1) - \frac{1}{2} s_1^2 h'(s_1) \right], \qquad |\mathbf{l}| = 1 , \tag{22}$$

$$\kappa = s_0^2 h(s_0), \qquad \mathbf{l} = \mathbf{0} . \tag{23}$$

Defining a new function,

$$g(s) = \frac{1}{2} s^2 h(s) , \tag{24}$$

Eqs. (21)–(23) are reduced to

$$\kappa = 2g(s_0), \qquad g(s_0) = g(s_1), \qquad g'(s_0) = g'(s_1) . \tag{25}$$

These relations (25) are in fact conditions on the choice of Hamiltonians, i.e., of the function $h(s)$. They are so far rather general, but we have to specify the values s_0, s_1. These values will be connected with the solution of (19) through the conditions (20), which actually constitute a linear equation,

$$\hat{L} u_{\mathbf{l}} = s_{\mathbf{l}} u_{\mathbf{l}} . \tag{26}$$

A solution to this equation can be cast into the form

$$u_{\mathbf{l}} = \int dq_1 \, dq_2 \cdots dq_d \times \frac{\cos(l_1 q_1) \cos(l_2 q_2) \cdots \cos(l_d q_d)}{2[\cos(q_1) + \cos(q_2) + \cdots \cos(q_d)] - s_1} , \tag{27}$$

where the integration extends for each variable q_i from $-\pi$ to π. Then the value for s_0 is given by

$$\frac{1}{s_0 - s_1} = \int dq_1 \, dq_2 \cdots dq_d \times \frac{1}{2[\cos(q_1) + \cos(q_2) + \cdots \cos(q_d)] - s_1} . \tag{28}$$

In other words, given the solution (27) to (19), we can generate the corresponding Hamiltonian by solving (25) with the additional constraint (28), which fixes the value s_0 relative to s_1. The function $g(s)$ can then be constructed in the following way: first choose s_1, then determine s_0, finally find a function $g(s)$ which is positive in s_1 and whose values and derivatives are equal in both s_0 and s_1. This function $g(s)$ will then define $h(s)$ with (24) and thus the Hamiltonian with potential energy (16).

Notice that (27) is exponentially localized around $\mathbf{l} = \mathbf{0}$ if $|s_1| > 2d$.

Conclusions.—We obtained explicit discrete breather solutions for several classes of Hamiltonian lattice models with different lattice dimensions. The outlined approach can be extended to other classes of lattice models with homogeneous potentials.

An interesting question for future studies will be the linear stability analysis of the obtained solutions, which is also closely related to the spectrum and character of small amplitude fluctuations around the state $x_l = 0$. Note that any solution which satisfies time-space separability can be continuously tuned to $x_l = 0$ by letting $A \rightarrow 0$ in (4), regardless of its spatial profile.

Finally one can extend the solutions of the site-ordered models to multisite breathers, for which

$$s_{\mathbf{l} \neq \mathbf{l}_m} = s_\infty, \qquad s_{\mathbf{l}_m} = s_m\,, \tag{29}$$

where the number of "defect" sites $\mathbf{l}_m$ is finite and the largest distance between any pair of "defect" sites is finite. Work is in progress.

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