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# Energy properties of discrete breathers

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**Abstract**

Discrete breathers are time-periodic, spatially localized solutions of equations of motion for classical degrees of freedom interacting on a lattice. They come in one-parameter families. We use recent results of Flach et al. (1997) on $d$-dimensional systems with local interaction and recent results of Gaididei et al. (1997) on one-dimensional systems with nonlocal interaction. We discuss energy properties of breathers in $d$-dimensional lattices with nonlocal interactions. Copyright © 1998 Elsevier Science B.V.

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## 1. Introduction

Recently progress has been achieved in the understanding of energy properties of localized excitations in nonlinear lattices. Discrete breathers (DBs) are time-periodic, spatially localized solutions of equations of motion for classical degrees of freedom interacting on a lattice [1–3]. The reason for the generic existence of DBs is the *discreteness of the system* paired with the *nonlinearity* of the differential equations defining the evolution of the system [4,5]. Thus one can avoid resonances of multiples of the discrete breather's frequency $\Omega_b$ with the phonon spectrum $\Omega_k$ of the system [6]. If the coupling is weak, the phonon spectrum consists of narrow bands. The nonlinearity and the narrowness of the phonon bands allows for periodic orbits whose frequency and all its harmonics lie outside the phonon spectrum. For some classes of systems, existing proofs of breather solutions have been published [7–9]. [2]

For generic Hamiltonian systems, periodic orbits occur in one-parameter families, and DBs are no exception. In many cases, the energy can be used as a parameter along the family, but as is well known, the energy can have turning points along a family of periodic orbits. Mathematically, such a turning point in energy is called a *saddle-centre periodic orbit*.

In a recent paper, Flach, Kladko and MacKay (FKM) [10] showed that in three-dimensional lattices, a turning point (in fact, minimum) in energy is almost inevitable for DB breather families. More specifically FKM gave heuristic arguments that the energy of a DB family has a positive lower bound for lattice dimension $d$ greater than or equal to some $d_c$, whereas for $d < d_c$ the energy goes to zero as the amplitude goes to zero, and confirmed these

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predictions numerically. The critical dimension $d_c$ depends on details of the system but is typically 2 and never greater than 2. Furthermore, for $d > d_c$ the minimum in energy occurs at positive amplitude and finite localization length. Notice that these studies have been done exclusively for systems with short range interaction (nearest neighbour interaction).

The reader might ask for a physical explanation of the existence of nonzero lower bounds on the breather energy. Since they were not given in FKM, let us mention here a possible way of argumentation. Consider a Hamiltonian system with an additional integral of motion – the norm (think of the discrete nonlinear Schrödinger equation as an example). Note that if the energy has a turning point on the breather family, so does the norm (because for small amplitudes and phonon band-edge wave vectors the two forms are quadratic and coincide, and both can be designed to be nonnegative). Suppose we consider the semiclassical regime of the corresponding quantum problem. The quantization of the norm leads to the number $N$ of quantum particles interacting through a potential which is given by the original nonlinear terms of the equations of motion. The breather solution corresponds to bound states of the quantum Hamiltonian with $N$ particles. The existence of a nonzero lower bound on the number of particles for bound states can be then explained as follows. According to our assumption we are working in the semiclassical regime, i.e. $N$ is large. Consider one quantum particle in the field of all other $N-1$ particles. Our tagged particle will feel a mean field (potential) caused by the presence of all other particles. In a bound state these particles cluster in a given part of the space. Depending on the sign of the interaction (i.e. of the original nonlinear term) the tagged particle will be either attracted by or repelled from the cloud of the other particles. The discreteness of the space ensures that these cases are essentially equivalent – because the kinetic energy of the particles (i.e. the original phonon band) is bounded from both sides (because the discretization of space leads to a cutoff in the wave vectors and thus to upper bounds of the phonon spectrum or kinetic energy). As is known, the existence of a bound state (for our tagged particle) in a potential well depends on the dimension of the space: for one- and two-dimensional systems bound states appear for any well, whereas in three dimensions a critical nonzero depth of the well is needed in order to produce a bound state. The depth of the well is roughly proportional to the number of the other particles. Consequently in three-dimensional systems a nonzero lower bound on the number of particles exists which is necessary in order to obtain a bound state of our tagged particle. Since the consideration does not depend on what particle has been tagged, the lower bound on the number of particles applies to the existence of the $N$-particle bound state as well. This result has been found already by Kosevich et al. (Section 10 of [11]). Note that it is not trivial to extend this result to systems with fluctuating particle numbers, i.e. for systems without norm conservation.

Another recent study of Gaididei, Mingaleev, Christiansen and Rasmussen (GMCR) [12] deals with the case of one-dimensional lattices with nonlocal dispersive interaction. This work shows how to obtain the dispersion relation for small wave numbers and thus Green's function in real space, which describes the spatial variation of solitary solutions.

In the present contribution we will combine both approaches to predict the energy properties of DBs in $d$-dimensional lattices with nonlocal interaction. Given the convergence of certain sums and the existence of DBs, we predict that the energy properties of DBs change drastically upon variation of the interaction range.

## 2. The case of nearest neighbour interaction

Let us consider a $d$-dimensional hypercubic lattice with $N$ sites. Each site is labelled by a $d$-dimensional vector $l \in Z^d$. Assign to each lattice site a state $X_l \in R^f$, where $f$ is the number of components and is to be finite. The evolution of the system is assumed to be given by a Hamiltonian of the form

$$H = \sum_l H_{\mathrm{loc}}(X_l) + H_{\mathrm{int}}(X_l, \{X_{l+l_0}\}), \qquad (1)$$

where $H_{\mathrm{int}}$ depends on the state at site $l$ and the states $X_{l+l_0}$ in a neighbourhood. We assume that $H$

has an equilibrium point at $X_l = 0$, with $H(\{X_l = 0\}) = 0$.

DB solutions come in one-parameter families. The parameter can be the amplitude (measured at the site with maximum amplitude), the energy $E$ or the breather frequency $\Omega_b$. It is anticipated (and was found both numerically and through some reasonable approximations [11]) that the amplitude can be lowered to arbitrarily small values, at least for some of the families for an infinite lattice. In this zero amplitude limit, the DB frequency $\Omega_b$ approaches an edge of the phonon spectrum $\Omega_k$. This happens because the nonresonance condition $\Omega_k/\Omega_b \neq 0, 1, 2, 3, \ldots$ has to hold for all solutions of a generic DB family [6]. In the limit of zero amplitude, the solutions have to approach solutions of the linearized equations of motion, thus the frequency $\Omega_b$ has to approach some $\Omega_k$, but at the same time not to coincide with any phonon frequency. This is possible only if the breather's frequency tends to an edge $\Omega_E$ of the phonon spectrum in the limit of zero breather amplitude. If we consider the family of nonlinear plane waves which yields the corresponding band edge plane wave in the limit of zero amplitude $A$, then its frequency $\Omega$ will depend on $A$ like

$$|\Omega - \Omega_E| \sim A^z \tag{2}$$

for small $A$, where the "detuning exponent" $z$ depends on the type of nonlinearity of the Hamiltonian (1), and can be calculated using standard perturbation theory [13].

An analysis of stability of band edge plane waves was carried out in [14] for systems with detuning exponent $z = 2$ and large $N$. The critical amplitude $A_{rmc}$ of the plane waves at the bifurcation point depends on the number of lattice sites as $A_c \sim N^{-1/d}$ [14]. We see that the amplitudes of the new orbits bifurcating from the plane wave become small in the limit of large system size. If the energy of the system is given by a positive definite quadratic form in the variables $X$ in the limit of small values of $X$, it follows for the critical energy of the plane wave at the bifurcation point [14]

$$E_c \sim N^{1-2/d}. \tag{3}$$

Result (3) is surprising, since it predicts that for $z = 2$ the energy of a DB for small amplitudes should diverge for an infinite lattice with $d = 3$ and stay finite (nonzero) for $d = 2$, whereas if $d = 1$, the breather energy will tend to zero (as initially expected) in the limit of small amplitudes and large system size.

We can estimate the DB energy in the limit of small amplitudes and compare the result with (3). Define the amplitude of a DB to be the largest of the amplitudes of the oscillations over the lattice. Denote it by $A_0$ where we define the site $l = 0$ to be the one with the largest amplitude. The amplitudes decay in space away from the breather centre, and by linearizing about the equilibrium state and making a continuum approximation, the decay is found to be given by $A_l \sim CF_d(|l|\delta)$ for $|l|$ large, where $F_d$ is a dimension-dependent function

$$F_1(x) = e^{-x}, \quad F_3(x) = \frac{1}{x}e^{-x}, \tag{4}$$

$$F_2(x) = \int \frac{e^{-x\sqrt{1+\zeta^2}}}{\sqrt{1+\zeta^2}}\, d\zeta, \tag{5}$$

$\delta$ is a spatial decay exponent to be discussed shortly, and $C$ is a constant which we shall assume can be taken of order $A_0$. To estimate the dependence of the spatial decay exponent $\delta$ on the frequency of the time-periodic motion $\Omega_b$ (which is close to the edge of the linear spectrum) it is enough to consider the dependence of the frequency of the phonon spectrum $\Omega_k$ on the wave vector $k$ when close to the edge. Generically this dependence is quadratic $(\Omega_E - \Omega_k) \sim |k - k_E|^2$ where $\Omega_E \neq 0$ marks the frequency of the edge of the linear spectrum and $k_E$ is the corresponding edge wave vector. Then analytical continuation of $(k - k_E)$ to $i(k - k_E)$ yields a quadratic dependence $|\Omega_b - \Omega_E| \sim \delta^2$. Finally we must insert the way that the detuning of the breather frequency from the edge of the linear spectrum $|\Omega_b - \Omega_E|$ depends on the small breather amplitude. Assuming that the weakly localized breather frequency detunes with amplitude as the weakly nonlinear band edge plane wave frequency this is $|\Omega_b - \Omega_E| \sim A_0^z$. Then $\delta \sim A_0^{z/2}$.

Now we are able to calculate the scaling of the energy of the DB as its amplitude goes to zero by replacing the sum over the lattice sites by an integral

$$E_b \sim \frac{1}{2} C^2 \int r^{d-1} F_d^2(\delta r)\,\mathrm{d}r \sim A_0^{(4-zd)/2}. \tag{6}$$

This is possible if the breather persists for small amplitudes and is slowly varying in space. We find that if $d > d_c = 4/z$, the breather energy diverges for small amplitudes, whereas for $d < d_c$ the DB energy tends to zero with the amplitude. Inserting $z = 2$ we obtain $d_c = 2$, which is in accord with the exact results on the plane wave stability [14] and thus strengthens the conjecture that DBs bifurcate through tangent bifurcations from band edge plane waves. Note that for $d = d_c$ logarithmic corrections may apply to (6), which can lead to additional variations of the energy for small amplitudes.

An immediate consequence is that if $d \geq d_c$, the energy of a breather is bounded away from zero. This is because for any nonzero amplitude the breather energy cannot be zero, and as the amplitude goes to zero the energy goes to a positive limit ($d = d_c$) or diverges ($d > d_c$). Thus we obtain an energy threshold for the creation of DBs for $d \geq d_c$. This new energy scale is set by combinations of the expansion coefficients in (1). These predictions were tested numerically and found to be correct [10].

## 3. Nonlocal interactions

Consider now a nonlocal interaction where $l_0$ can become infinite in (1):

$$H_{\text{int}} = \frac{C}{2} \sum_{m \neq l} \frac{1}{|m-l|^s} (X_l - X_m)^2. \tag{7}$$

This interaction has been considered in [12] for a cubic nonlinear Schrödinger chain. In the following I will sketch the results of GMCR with regard to energy properties for the case $d = 1$.

First we need the dispersion relation of (7) for small wave numbers $k$. For simplicity assume the equations of motion to be of the form $\ddot{X}_l = -\partial H / \partial X_l$ and $H_{\text{loc}} = X^2/2$ for small values of $X$. Then the dispersion relation for (1) with (7) reads

$$\Omega_k^2 = 1 + 2C \sum_{m=1}^{\infty} \frac{1 - \cos(km)}{m^s}. \tag{8}$$

The squared plane wave frequency $\Omega_k^2$ is given by a Dirichlet L-series, where the sum in (8) converges for $s > 1$. Further $0 \leq (\Omega_k^2 - 1) \leq 4C\zeta(s)$, where $\zeta(s)$ is the Riemann Zeta function. Obviously $\Omega_k^2(k = 0) = 1$. To derive the dependence of $\Omega_k^2$ on $k$ for small wave numbers we first consider the case $1 < s < 3$. In this case the sum can be replaced by an integral for small $k$:

$$f_s(k) = \sum_{m=1}^{\infty} \frac{1 - \cos(km)}{m^s} = a(s) k^{s-1},$$
$$a(s) = \int_0^{\infty} \frac{1 - \cos x}{x^s}\,\mathrm{d}x. \tag{9}$$

For the integral $a(s)$ to converge we need $s > 1$ (upper integration boundary) and $s < 3$ (lower integration boundary). For $s > 3$ we can use the identity $\partial^2 f_s(k)/\partial k^2 = -f_{s-2}(k) + \zeta(s-2)$. Indeed for $3 < s < 5$ and small $k$ we find $f_s(k) = \zeta(s-2)k^2/2 + O(k^{s-1})$. The same procedure can be applied to all larger values of $s$, so that finally we obtain for small $k$:

$$\Omega_k^2 = 1 + C\zeta(s-2)k^2 \quad (s > 3),$$
$$\Omega_k^2 = 1 + 2Ca(s)k^{s-1} \quad (1 < s < 3). \tag{10}$$

Now we calculate Green's function

$$G_\lambda(n) = \int \frac{\cos(kn)}{\lambda^2 + \Omega_k^2 - 1}\,\mathrm{d}k \tag{11}$$

for large values of $n$ [12]:

$$G_\lambda(n) \sim \mathrm{e}^{-\lambda n} \quad (s > 3)$$
$$G_\lambda(n) \sim n^{-s} \quad (1 < s < 3). \tag{12}$$

A DB with frequency $|\Omega - \Omega_E| = \lambda$ will have a spatial decay in its tails governed by (12). Clearly the dimension-dependent $F_d$ functions from the previous section can be obtained in precisely the same way for $s \to \infty$.

Assuming again that the breather solution can be continued down to small amplitudes where the parameter $\lambda$ becomes small we can estimate the energy dependence on the amplitude. For $s > 3$ the spatial decay of the breather is exponential – as in the case $s \to \infty$

for the nearest neighbour interaction. The exponent of this decay is $\lambda$ dependent. This dependence allows for qualitatively different $E_b(A)$ behaviour depending on the type of nonlinearity (note that we still consider $d = 1$) as given by (6). We thus can predict that the energy of a breather in a one-dimensional lattice will diverge for small amplitudes provided $s > 3$ and the nonlinearity is strong enough such that the detuning exponent $z \geq 4$. This will be the case e.g. for the quintic nonlinear Schrödinger chain with nonlocal interaction.

A different situation arises for $1 < s < 3$. Not only is the spatial decay now algebraic, but also the exponent of the decay does not depend on the breather parameter $\lambda$ anymore. Consequently the energy of the breather will be a quadratic function of the breather amplitude for small amplitudes. Even if the nonlinearity is strong enough such that for $s > 3$ $E_b$ diverges for small amplitudes, the energy decays to zero for $1 < s < 3$ and small amplitudes. Consequently we expect the nonzero bounds on the breather energy to disappear regardless of what the nonlinear terms might yield for $s > 3$.

## 4. Higher lattice dimensions

Now we generalize the findings to higher lattice dimensions. For the case $s \to \infty$ (nearest neighbour interaction) we already found that a critical dimension $d_c$ exists such that for $d > d_c$ the breather energy will be always bounded away from zero. This fact relies on the circumstance that the exponent of the spatial decay governing the breather variation in space depends on the breather parameter (frequency or amplitude). What can be expected for nonlocal interaction when $s$ is finite?

To proceed we first need the dispersion relation. We consider again a hypercubic lattice of dimension $d$ and spacing one. Then the dispersion is given by

$$\Omega_k^2 = 1 + 2C \sum_{\nu} \frac{1}{a_\nu^s} \sum_{m=1}^{\infty} \frac{1 - \cos(k_\nu m)}{m^s},$$

$$k_\nu = k a_\nu \cos\phi_\nu, \quad a_\nu = \sqrt{\sum_{\mu=1}^{d} p_\mu^2}. \tag{13}$$

Here the integers $p_\mu$ have to fulfill the condition $\{p_1, p_2, \ldots, p_d\} = 1$ (largest common divisor equals one). The angle $\phi_\nu$ is spanned by the wave vector $\mathbf{k}$ and the lattice vector $\mathbf{p}_\nu$. The double sum in (13) converges if $s > 1$ and if the sum $\sum_\nu 1/a_\nu^s$ converges. Since $a_\nu^2$ is an integer, this sum certainly converges if $s > 2$. Most probably it will converge even for $s > 1$ but this demands a separate proof.

Let us give a comment on how to derive (13). The idea is to choose a lattice site $l = 0$, and to consider the sum over all other sites in the interaction hamiltonian as a double sum: the inner sum goes over a chain with spacing $a_\nu$ and wave vector $k_\nu$. The outer sum goes over all such 'irreducible' chains. The angle dependence enters through the effective wave vector $k_\nu$.

Now we can first evaluate the inner sums. For small $k$ values we again find $\Omega_k^2 - 1 \sim k^2$ for $s > 3$ and $\Omega_k^2 - 1 \sim k^{s-1}$ for $2 < s < 3$. Keeping in mind that the full dispersion relation will depend on some angles, the dependence on the absolute value of the wave vector is found to coincide with the one-dimensional case.

Consequently the spatial decay of the breather for $s > 3$ is given by (4) and (5). Again we obtain that the energy of the breather is bounded away from zero provided $d > d_c$.

For $2 < s < 3$ the situation is again different. The spatial decay of the breather is algebraic – e.g. for $d = 3$ it will be proportional to $1/r^{s+1}$. But the main point is that the exponent will not depend on the breather parameter. Consequently the energy of the breather should vanish in the limit of small amplitudes.

## 5. Discussion and summary

Let us discuss similarities and differences of the obtained results with the scaling theory for polarons for one electron interacting with a classical deformable lattice following the work of Emin and Holstein [15] (see also [16]). The ground state of such a system is given by a static lattice deformation $\Delta(\mathbf{r})$ and a corresponding one-electron wave function $\Psi(\mathbf{r})$ (note that minimization with respect to the strain field yields a functional dependence of $\Delta(\mathbf{r})$ on $\Psi(\mathbf{r})$). The idea of Emin and Holstein was to replace the yet unknown true groundstate wave function by a scaled function $R^{-d/2}\Psi(\mathbf{r}/R)$ keeping the normalization condition. Considering the groundstate energy $E(R)$ as a function of $R$, the condition on starting with the true groundstate is that $E(R)$ shows a minimum. Formally that should be at $R = 1$. However if we find a minimum in $E(R)$ at $R \neq 1$, then we simply rescale all coordinates. So we have to see whether $E(R)$ admits nontrivial minima at all. Emin and Holstein considered among others a local electron–lattice interaction. This yields a continuum Nonlinear Schrödinger dependence of $E(\Psi)$ and the dependence $E(R) = T/R^2 - V^s/R^d$, where $T$ is the kinetic energy of the electron, and $V^s > 0$ is the interaction energy. For $d = 3$ $E(R)$ shows a minimum at $R = \infty$, a maximum at some finite $R_{\max}$ and a divergence to $-\infty$ at $R = 0$. Within the framework of polaron theory one arrives at the conclusion that a small polaron exists, with size zero within the continuum approach (the ultraviolet divergence is stopped upon discretization of space, i.e. the small polaron should have a size comparable to the interatomic distance). Within the continuum approach this small polaron has an infinite binding energy, which again becomes finite only after discretizing space (see e.g. [17], where the effects of discreteness are studied for $d = 2$). Finally we could consider different values of the charge. Trivially these lead only to a rescaling of the ratio $T/V^s$.

What is the similarity to breathers? First in the specific case of a nonlinear Schrödinger equation a continuous gauge transformation can map any time-periodic solution into a static solution of a rescaled nonlinear Schrödinger equation. Second static solutions are extrema of the energy. Thus all extrema of the function $E(R)$ from above can be considered as classical breather solutions of the nonlinear Schrödinger equation. The extremum at $R = 0$ is the well-known collapse solution [18]. For the same norm we find another breather solution which is unstable (corresponding to the maximum in $E(R)$). This is similar to our findings, because instead of considering the energy we could as well consider the action of a breather orbit, or the norm for the nonlinear Schrödinger case.

However from our consideration it follows that no breathers exist upon lowering the energy/action/norm below a nonzero threshold. This is evidently not the case for the continuum polaron. The continuum version will always provide with a small polaron solution. Apparently the discreteness of the underlying space is relevant for this result [19]. This is also confirmed by the numerical study in [10] where the minimum energy breather was found to be localized on a few lattice sites. What is known from perturbation theory on the lattice is that for the groundstate to be polaronic it needs to overcome a finite threshold in $V^s$ which is equivalent to a finite threshold in the norm. But this result does not tell that the extremum associated with the polaron disappears at some different threshold value of $V^s$. Apparently our result provides also this conclusion, although in the context of polaron theory this is of minor interest. Further differences are due to the fact that when considering breather properties we are not confined to systems which conserve a norm. In the language of polarons this corresponds to considering additional terms which do not conserve the number of electrons. To conclude this discussion we believe that there are several similarities between what is known as polaron scaling theory and our results on breather properties. But the results for breathers, which are obtained using a small number of input assumptions, can only be guessed when staying on the ground of standard continuum polaron scaling theory.

In conclusion we have extended the analysis of breather energy properties to the case of nonlocal interaction and higher lattice dimensions. A number of assumptions are entering this analysis. The breather should be continuable to small amplitudes, where its frequency should come close to the phonon band. Then for interactions decaying faster than dipole–dipole interaction ($s > 3$) the breather shows exponential decay in space, and its energy is bounded away from zero provided the lattice dimension is larger than a critical one (which depends on the type of nonlinearity and can be even equal to one). For $2 < s < 3$ the breather decays algebraically in space, and the energy threshold for creating a breather is zero, independent of the lattice dimension (for $d = 1$ this result extends to values $1 < s < 3$). Note that this follows not simply from the type of the spatial decay (exponential versus algebraic), but rather from the dependence or independence of the exponent of the decay on the breather parameter.

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