Localized excitations and their thresholds

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(Received 4 August 1999)

We propose a numerical method for identifying localized excitations in discrete nonlinear Schrödinger type models. This methodology, based on the application of a nonlinear iterative version of the Rayleigh-Ritz variational principle yields breather excitations in a very fast and efficient way in one or higher spatial dimensions. The typical convergence properties of the method are found to be super-linear. The usefulness of this technique is illustrated by studying the properties of the recently developed theoretical criteria for the excitation power thresholds for nonlinear modes.

PACS number(s): 45.10.−b, 63.20.Pw

In recent years, an increasing number of studies have been devoted to the study of localized excitations in nonlinear lattices [1]. This growing interest is based on the fact that the proven existence [2] of such modes suggests a tempting explanation of energy focusing, important to many branches of physics. Also, more recently there has been some theoretical speculation on the compatibility of such modes with the breathing oscillations of the DNA double strand [3] and the behavior of the amorphous materials [4]. Even more importantly, in the past year, there has been strong experimental evidence for the existence of such modes in certain electronic materials, as revealed through Raman spectroscopy [5].

In this light, we will, in this paper, propose a technique for numerically constructing breathers, and utilize it to clarify a number of theoretical aspects. The main thrust of this study will be the construction of breathers in the context of the discrete nonlinear Schrödinger (DNLS) equation. This model has wide applicability, ranging from biology and condensed matter physics to nonlinear optics [6]. Furthermore, it is of importance in, practically, every application that can be modeled by a Klein-Gordon (KG) type of nonlinear lattice equation, since the envelope of nonlinear KG waves is governed to leading order by the DNLS equation.

The methodology we propose is based on the gauge symmetry of the DNLS equation and hence the essential ingredient is its monochromatic nature. More explicitly, seeking solutions of the form $\exp(-i\omega t)u_i$ to the equation

$$i\dot{\psi}_i = -k(\psi_{i+1} - 2\psi_i + \psi_{i-1}) - |\psi_i|^{2\sigma}\psi_i, \tag{1}$$

one arrives at a nonlinear eigenvalue problem determining the the spatial envelope profile $\{u_i\}$,

$$\omega u_i = -k(u_{i+1} - 2u_i + u_{i-1}) - |u_i|^{2\sigma}u_i. \tag{2}$$

Inspired by Ref. [7], we can view the equation for u_i as a bound state quantum-mechanical problem, $\hat{H}\vec{u} = \omega\vec{u}$. However, instead of a linear Schrödinger operator, we have a nonlinear discrete operator $\hat{H}$ whose bound states (lowest energies) will be the localized excitations whose properties we are studying. Due to its nonlinear nature (the diagonal entries of the matrix $[H]_{ii} = 2k - |u_i|^{2\sigma}$ depend on the eigenvector), a direct solution of the eigenvalue problem is not available. It is possible however to search *iteratively* for a solution of the eigenvalue equation. This is reminiscent of the Rayleigh-Ritz principle in linear quantum mechanics, where the expectation value $\langle u|H|u\rangle$ of any normalized state gives an upper bound for the energy of the ground state that one is looking for. Explicitly the idea is that, based on an initial guess used in the operator $\hat{H}$, one solves the resulting linear eigenvalue problem and uses the result in recalculating $\hat{H}$ and so on, until desired precision is reached. Methods of similar nature have previously been used in the study of the Holstein polaron model, and similar problems [8].

Some previously applied construction techniques deal with the full time-dependent problem and are based either on continuation techniques [9,10] or on limit-cycle techniques with good initial guesses [11]. These methods require full scale time integration until the trajectory returns to the Poincaré section (essentially in one time period of the breather oscillation) and subsequent refinement of the spatial structure through a Newton iteration. Such methods are evidently very time consuming. The advantage of such methods is that one can solve, coupled to the direct full-scale time integration, the variational equations for the dependence of the final state on the initial state (see, i.e., Refs. [9] and [11]) and thereby determine the stability in terms of Floquet multipliers. However, for the DNLS equation construction and stability information can be achieved in several alternative ways [12]. For purely construction purposes, however, our technique is much less time intensive, and much more robust in cases where the Newton iteration may encounter problems (i.e., when an extra Floquet multiplier approaches unity). In most of the cases we have studied the convergence of the method is superlinear.

One of the important assets of our method is that it hinges on the solution of eigenvalue problems for *sparse* matrices. Basically only the diagonal and principle off diagonals are populated. Hence, it is easy to implement special algorithms developed for matrices with this sort of symmetric sparse structure to significantly reduce the amount of required computations, which is important in higher dimensions.

As an illustration of our method's value, we will in the following present one-dimensional calculations where the

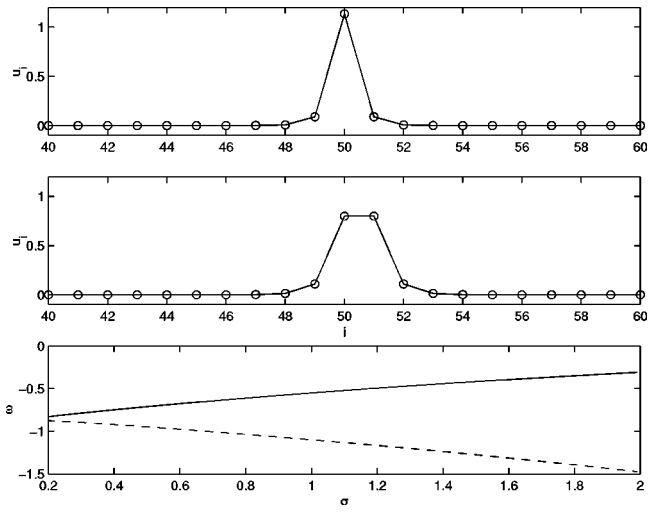

FIG. 1. Envelope profile u_i of an odd and an even mode constructed by our method for $P=1.3$ (top two panels). Bottom panel shows bound state eigenvalues for the even (solid line) and the odd (dashed line) modes (see text).

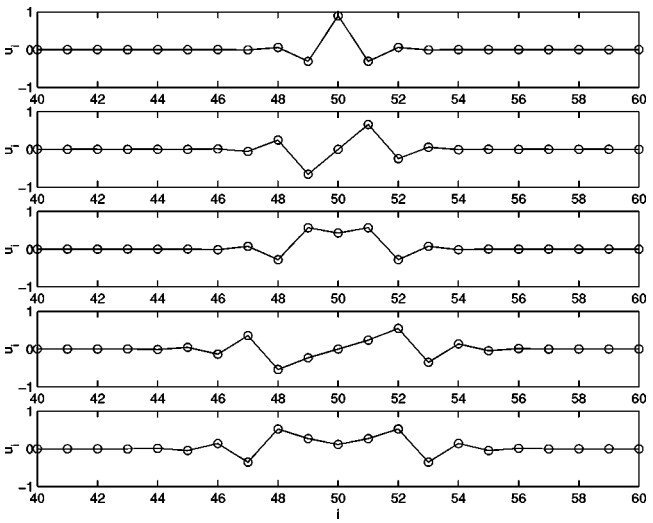

FIG. 2. The ground and first four excited odd localized staggered states existing for very small values of the nonlinearity parameter σ. Here, $\sigma=0.15$.

strength of the nonlinearity parameter σ is varied while the coupling is fixed. The way to construct breathers of any prescribed power, $P=\Sigma_i|\psi_i|^2$, for a definite value of σ, is, at every step of the iteration, to scale the computed normalized eigenvector as $u_i \rightarrow P^{1/2}u_i$.

Depending on the initial condition and the center position, we can normally trace breathers centered on a site (odd modes) or centered between sites (even modes). An example of two modes with the same power ($P=1.3$) for the two cases is given in the top two panels of Fig. 1.

From previous studies it is well known that the even and odd modes do not possess the same energy, resulting in an ''effective'' Peierls-Nabarro (PN) barrier [14,15]. As is known by analytical methods [15], for the unstaggered case the odd mode is the real ground state and the unstable even mode will eventually collapse to it. Hence, we anticipate that as we increase the value of the nonlinearity parameter, the odd modes will always correspond to a more negative eigenvalue (for the same power) confirming the above stability features. This is what we observe in the bottom panel of Fig. 1, showing the even and odd mode eigenvalues. The eigenvalues merge in the linear case (since the absence of nonlinearity degenerates the states, making them extended) but as σ is progressively increased, the height of the ''effective'' PN barrier becomes larger and the excitations concentrate on a single site (as predicted in Ref. [7]).

Another important trait of this technique is that it can always probe how many localized modes exist on the lattice. For large values of the nonlinearity parameter σ (when looking for a specific kind of mode, say, even) there will appear one bound state or none (beyond the threshold σ for the predefined power), while for small values of σ emerging from the linear limit of extended excitations, there will appear many localized modes that can be probed through the eigenvalues of the matrix. In this way, one can probe not only the ground state of the problem, but also the excited states that correspond to the rest of negative (bound state) eigenvalues of the problem. Our linear stability results for such modes within the framework of the rotating wave approximation indicate that in the case of even parity, they typically correspond to local minima of the energy whereas for odd parity solutions, they typically correspond to saddle points. Our stability calculations will be analyzed in more detail elsewhere [13]. A typical search of such excited states in the case of staggered odd modes for $\sigma=0.15$, $k=0.1$, $P=1.0$ appears in Fig. 2. The eigenfunction corresponding to the five most negative eigenvalues are shown in the figure. This picture is reminiscent of multiple localized modes observed in Ref. [14]. Our results indicate that such states exist only for $\sigma<0.5$ and they can be continued to the uncoupled limit where a relation to multibreather configurations can be established [13].

Generalization to d dimensions is very straightforward [16]. Then, one deals with an $N^d \times N^d$ sparse matrix, which has the same structure as before in the diagonal and principal off diagonal bands but has also been filled in the band of elements $[H]_{m,m+nN}$, $n=1,\ldots,d-1$. This is, of course, true for fixed boundary conditions (BC). The implementation of periodic BC follows directly by adding $[H]_{1,nN}=-k_i$, $[H]_{nN,1}=-k_j$, with $n=1,\ldots,d$ (k_i and k_j are defined in Ref. [16]). In this way, we can easily construct unstaggered breathers, such as those shown in Ref. [18], but also staggered in any direction (i.e., as shown in Fig. 3 for two dimensions) localized excitations in two or higher dimensions.

In order to demonstrate the accuracy of our method we have extended it to nonlinear KG chains. Taking a typical such example [7,17]

$$\ddot{u}_i = D(u_{i+1}+u_{i-1}-2u_i)-\Omega^2 u_i+u_i^3 \qquad (3)$$

and looking for a perturbative solution to leading order $u_i=\epsilon\Psi_i$, with $\Psi_i=\exp(-i\Omega t)\psi_i+\exp(i\Omega t)\psi_i^*$, rescaling $D \rightarrow \epsilon^2 k$, we get an equation (in rescaled time $t'=\epsilon^2 t$) which reads $i\Omega\dot{\psi}_i=-k(\psi_{i+1}-2\psi_i+\psi_{i-1})-3|\psi_i|^2\psi_i$. Through this derivation, solutions valid to times $O(\epsilon^{-2})$ are obtained. Checking this (as well as the accuracy of our construction technique), we have used the DNLS approximation to con-

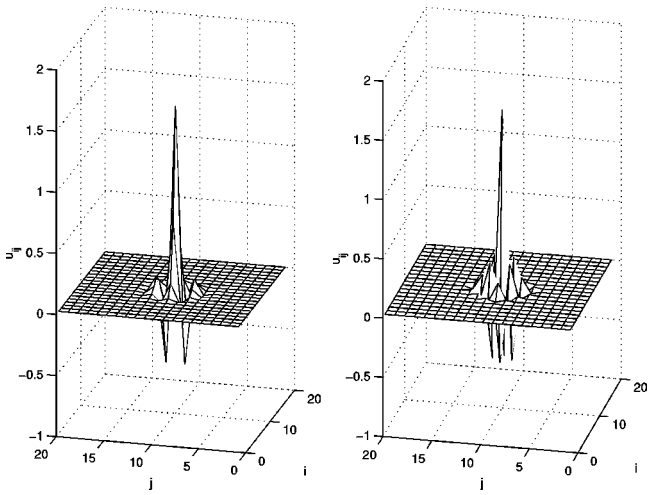

FIG. 3. Profile of a two-dimensional breather staggered along one (left panel, $k_i=-k_j=0.1$) or both (right panel, $k_i=k_j=-0.1$) directions; $\sigma=1$.

struct breathers, subsequently input to integrators of the above KG equation. The result is plotted in Fig. 4 for an even mode.

We can see that the mode is propagating essentially unaltered throughout our simulation. At large time scales, this solution, as expected, will eventually get reshaped into a stable localized odd mode.

One of the powerful indications of the usefulness of our technique is its ability to calculate the excitation thresholds of breathers. The discussion of these power (or energy) thresholds was initiated for the DNLS in Ref. [18] (although already known for polarons [19]), where a scaling argument was used to show that the power (energy in the terminology of Ref. [18]) of a localized breather excitation will be $P \sim A^{2-d\sigma}$ with A the amplitude of the excitation and d the dimension of the lattice. Hence, for $\sigma<2/d$ there exist breathers of arbitrarily small power. On the other hand, if $\sigma \geqslant 2/d$, then for the equality the energy approaches a constant and for the inequality, it diverges as A tends to zero. Hence, there cannot exist breathers of arbitrarily small energy, indicating the existence of a threshold.

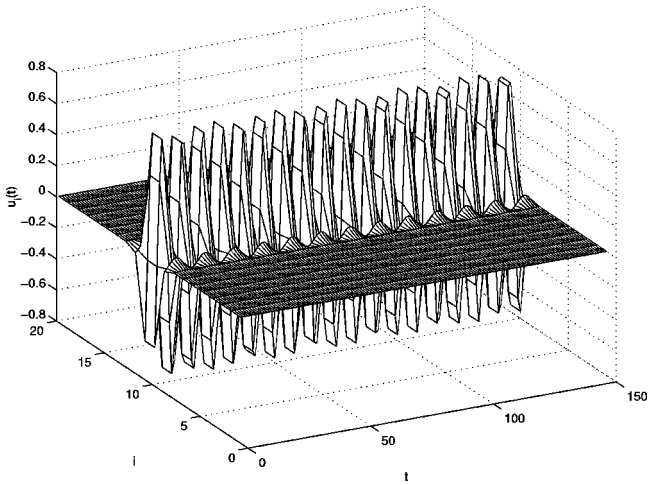

FIG. 4. Propagation of unstable KG breather (constructed through our technique).

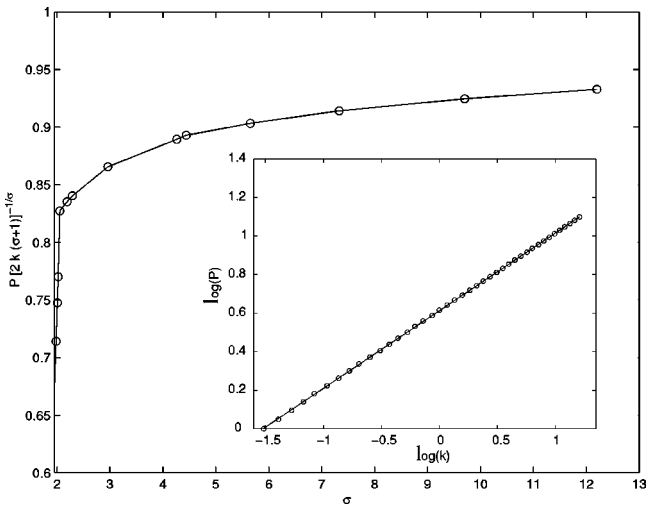

FIG. 5. Plot of the excitation threshold for $f=P[2k(\sigma+1)]^{-1/\sigma}$, as a function of the nonlinearity parameter σ. Inset shows log-log plot of the threshold power for breather excitations as a function of coupling strength, for fixed $\sigma=2.5$.

Very recently, Weinstein [7] was able to prove this conjecture rigorously using essentially a Rayleigh-Ritz formulation of the nonlinear eigenvalue problem that is used here, in conjunction with the Nirenberg inequality [20]. Weinstein was able to prove that the excitation power threshold has the functional form

$$P_{thresh}=[(\sigma+1)kI]^{1/\sigma}, \tag{4}$$

where

$$I=\inf \frac{\left(\sum_i |u_i|^2\right)^{\sigma} \sum_i [-u_i(u_{i+1}+u_{i-1}-2u_i)]}{\sum_i |u_i|^{2\sigma+2}}. \tag{5}$$

Our contribution (and at the same time an excellent cross check of both our technique as well as of the validity of the theoretical results developed in Ref. [7]), is to perform numerical studies to explicitly calculate the power threshold as a function of the coupling parameter k as well as the nonlinearity parameter σ.

Finding the power thresholds using our numerical scheme can be approached in two ways. We can find the minimum power for which an excitation can survive in a lattice with a particular strength of coupling or nonlinearity. Alternatively, we can search for the maximum σ or k that can sustain breathers of a certain power.

Our results are summarized in Fig. 5. The inset shows a log-log plot of the power P versus the coupling k for a fixed value of the nonlinearity parameter $\sigma=2.5$. In extremely good agreement with the theoretical prediction of Ref. [7] of a linear correspondence with a slope of $1/\sigma=0.4$, we find a slope $S=0.403$. The same kind of agreement was observed in all the cases tested for the dependence of P on k. The figure also shows for a fixed value of the coupling ($k=0.1$) the dependence of a theoretically motivated function $f=P[2k(\sigma+1)]^{-1/\sigma}$ on σ. Our motivation in selecting this combination of axes is in order to verify the validity of our

results in the large σ limit. In that limit using the argument of the localization of the excitation on a single site it can be readily seen that $\lim_{\sigma\to\infty} I=2$. Hence, $\lim_{\sigma\to\infty} f=1$, again in very good agreement with our results. An important product of this calculation, is the behavior of f at small values of the nonlinearity parameter, where the limit calculations do not apply. We can see that the dependence of I on σ departs from the predicted threshold of 2 [the simulations are in one dimension (1D)] and is replaced by a sharp increase, before single site localization takes over, leading towards the limit dependence illustrated above.

In summary, we have presented a numerical method for the construction of discrete, localized, time periodic modes supported by nonlinear lattices subject to Hamiltonian dynamics. A clear asset of the method is its very straightforward numerical implementation and the ability to use sparse matrix eigenvalue solvers, significantly reducing the number of computations, and facilitating the generalization of the approach to higher dimensions for large lattices. In the setup of the nonlinear matrix eigenvalue problem, the theoretical background of such a generalization is quite simple, as we have indicated. Importantly, we have used this method to quantitatively predict the behavior of the threshold of these breather excitations, conjectured in Ref. [18] and predicted in Ref. [7]. Not only has excellent agreement been established with the theoretical predictions of Ref. [7], but in fact the method has rendered possible the numerical exploration of regimes of parameter space that were not amenable to analytical treatment.

We believe that our findings will permit the theorist to construct, probe and understand better the nature of such modes and their properties. The experimentalist will have a quantitative and straightforward tool for predicting the thresholds of excitations of these modes, in realistic, experimental situations.

P.G.K. gratefully acknowledges support from the ''Alexander S. Onasis'' Public Benefit Foundation. Research at Los Alamos National Laboratory is performed under the auspices of the U.S. DOE.

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