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Mobile localization in nonlinear Schrödinger lattices

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Abstract

Using continuation methods from the integrable Ablowitz–Ladik lattice, we have studied the structure of numerically exact mobile discrete breathers in the standard discrete nonlinear Schrödinger equation. We show that, away from that integrable limit, the mobile pulse is dressed by a background of resonant plane waves with wavevectors given by a certain selection rule. This background is seen to be essential for supporting mobile localization in the absence of integrability. We show how the variations of the localized pulse energy during its motion are balanced by the interaction with this background, allowing the localization mobility along the lattice.

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1. Introduction

The phenomenon of intrinsic localization (collapse to self-localized states) due to nonlinearity in discrete systems governed by Schrödinger equations is of fundamental interest in nonlinear physics [1,2], and is the subject of current active experimental research in several areas like nonlinear optics [3], Bose–Einstein condensate arrays [4–6], polaronic effects in biomolecular processes, and local (stretching) modes in molecules and molecular crystals (see [1,7,8] and references therein). Discrete nonlinear Schrödinger equations (NLS lattices for short) provide the theoretical description of these systems, where pulse-like (self-localized) states are observed.

The standard discrete nonlinear Schrödinger (DNLS) equation is the (simplest) discretization of the one-dimensional continuous Schrödinger equation

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with cubic nonlinearity in the interaction term, i.e.,

$$\mathrm{i}\dot{\Phi}_n = -(\Phi_{n+1} + \Phi_{n-1}) - \gamma|\Phi_n|^2\Phi_n, \tag{1}$$

where $\Phi_n(t)$ is a complex function of time. The first term on the right takes account of the dispersion and the second of the nonlinearity, the parameter γ is the ratio between them. For the Bose–Einstein condensate lattices dealt with in [4–6] one can think of Φ_n as the boson condensate wave function in the nth (optical) potential well, and γ would thus be related to the so-called s-wave scattering length [9]. The self-focussing effect of local nonlinearity balanced by the opposite effect of the dispersive coupling makes possible the existence of localized boson states in the Schrödinger representation of the condensate lattice (Gross–Pitaevskii equation). In a localized state (discrete breather) of the boson lattice the profile of $|\Phi_n|^2$ decays exponentially away from the localization center. These solutions have an internal frequency, $\Phi_n = |\Phi_n|\exp(\mathrm{i}\omega_b t)$, so that the discreteness is essential to avoid resonances with the phonon band and keeping localized the energy. Pinned (immobile) localized solutions of Eq. (1) have been rigorously characterized [10] and extensively studied by highly accurate numerical [11] and analytical approximations. However, for exact *mobile* discrete breathers no rigorous formal proof of existence in standard DNLS is available nowadays although lot of works have studied these kind of solutions (see, e.g., [12–15]).

The translational motion of discrete breathers introduces a new time scale (the inverse velocity) into play, so generically a moving breather should excite resonances with the plane wave band expectra. In a Hamiltonian system, these radiative losses would tend to delocalize energy and some compensating mechanism is needed in order to sustain exact stationary states of breather translational motion. To address the problem we use unbiased (i.e., not based on ansatze on the expected functional form of the exact solution) and precise numerical methods which allow observations of numerically exact nonintegrable mobility, paving the way to further physical (and mathematical) insights.

In this Letter, after explaining in Section 2 the basis of the numerical method (fixed point continuation from the integrable Ablowitz–Ladik limit [16]) and its relevant technical details briefly, we will discuss the structure of the discrete NLS breathers in Section 3. They are found to be the exact superposition of a travelling exponentially localized oscillation (the *core*), and an extended "background" built up of finite amplitude plane waves $A\exp[\mathrm{i}(kn - \omega t)]$. These resonant plane waves fit well simple (thermodynamic limit) predictions based on discrete symmetry requirements. Finally in Section 4 we show how the resonant background is seen to be an indispensable part of the solution. In this regard we present the mechanism through which the interaction core-background compensates the variations of the core energy (no longer an invariant of motion away from the integrable limit), during the translational motion.

2. Salerno model and continuation method

The method used here makes use of the following NLS lattice, originally introduced by Salerno [17],

$$\mathrm{i}\dot{\Phi}_n = -(\Phi_{n+1} + \Phi_{n-1})\big[1 + \mu|\Phi_n|^2\big] - 2\nu\Phi_n|\Phi_n|^2. \tag{2}$$

This lattice, though nonintegrable for $\nu \neq 0$, provides a Hamiltonian interpolation between the standard DNLS equation (1), for $\mu = 0$ and $\nu = \gamma/2$, and the integrable Ablowitz–Ladik lattice [16], AL for short, when $\mu = \gamma/2$ and $\nu = 0$. The AL model is a remarkable integrable lattice possessing a family of exact moving breather solutions:

$$\Phi_n(t) = \sqrt{\frac{2}{\gamma}}\sinh\beta\,\mathrm{sech}\big[\beta\big(n - x_0(t)\big)\big] \times \exp\big[\mathrm{i}\big(\alpha\big(n - x_0(t)\big) + \Omega(t)\big)\big], \tag{3}$$

the two parameters ω_b and v_b are the breather frequency and velocity

$$\omega_b \equiv \dot{\Omega}(t) = 2\cosh\beta\cos\alpha + \alpha v_b,$$
$$v_b \equiv \dot{x}_0(t) = \frac{2}{\beta}\sinh\beta\sin\alpha, \tag{4}$$

where $-\pi \leqslant \alpha \leqslant \pi$ and $0 < \beta < \infty$. Eq. (2) has the following conserved quantities, namely, the Hamiltonian H and the norm N:

$$H = -\sum_n(\Phi_n\bar{\Phi}_{n+1} + \bar{\Phi}_n\Phi_{n+1}) - 2\frac{\nu}{\mu}\sum_n|\Phi_n|^2 + 2\frac{\nu}{\mu^2}\sum_n\ln\big(1 + \mu|\Phi_n|^2\big), \tag{5}$$

$$N = \frac{1}{\mu} \sum_n \ln\bigl(1 + \mu|\Phi_n|^2\bigr), \tag{6}$$

where $\bar{\Phi}_n$ denotes the complex conjugate of Φ_n. In what follows we will fix the value $\gamma = 2$ in Eq. (1) and $\mu + \nu = 1$ in Eq. (2), as usual.

Perturbative inverse scattering transform [18], as well as collective coordinate methods [2,19,20], have been used to study moving breathers of the Salerno equation (2) near the integrable AL limit ($\nu \simeq 0$). The numerical procedure that we explain below has the advantage of being unbiased and not restricted to small values of the nonintegrability parameter ν, at the expense of restricting attention to those solutions (3) which are *resonant*, meaning that the two breather time scales are commensurate $2\pi v_b/\omega_b = p/q$ (rational time scales ratio). A resonant (p/q) moving breather $\hat{\Phi}_n(t)$ is numerically represented as a fixed point of the map $M = L^p T^q$, where L is the lattice translation operator $L(\{\Phi_n(t)\}) = \{\Phi_{n+1}(t)\}$, and T is the T_b-evolution map ($T_b = 2\pi/\omega_b$), $T(\{\Phi_n(t)\}) = \{\Phi_n(t + T_b)\}$, explicitly

$$\hat{\Phi}_n(t) = \hat{\Phi}_{n+p}(t + qT_b) \quad \text{for all } n. \tag{7}$$

Let us briefly present the numerical method. The implicit function theorem [21] ensures a unique continuation of a fixed point solution of M for parameter (ν) variations, provided the Jacobian matrix $J = D(M - I)$ is invertible: with this proviso the Newton method [22] is an efficient numerical algorithm to find the uniquely continued fixed point. In other words, continuation from a resonant AL breather along the Salerno model is possible if one restricts the Jacobian matrix J to the subspace orthogonal to its center (null) subspace. The center subspace turns out to be spanned by two continuous symmetries of the Salerno model, namely, *time translation* and *gauge* (uniform phase rotation) invariances. Using singular value decomposition (SVD) techniques [23], one then obtains numerically accurate continued resonant moving breathers along the Salerno model until conditions for continuation cease to hold. A (SVD)-regularized Newton algorithm was already used by Cretegny and Aubry in [12] to refine moving breathers of Klein–Gordon lattices with Morse potentials obtained by other means. From the methodological side what is novel here is the systematic use of it in order to obtain the family of moving Schrödinger breathers of the NLS lattice (2), for different values of $2\pi v_b/\omega_b = 0, 1/2, 3/4, 1, \ldots$ and a fine grid of frequency values ω_b and the nonintegrability parameter ν.

3. Mobile discrete breathers

Let first start with a few remarks on immobile breathers ($p = 0$). Some nonintegrable issues, that affect mobile solutions, can be shown continuing the immobile ones along the Salerno model ($\nu = 0, \ldots, 1$). First we remark that the uniquely continued solution of standard DNLS ($\nu = 1$) is equal to the pinned discrete breather uniquely continued from the anticontinuous limit ($\gamma \to \infty$) [10]. Second, only inmobile breathers which are centered either at a site (n) or at a bond ($n \pm 1/2$) persist; this is due to the emergence of Peierls–Nabarro barriers away from integrability ($\nu \neq 0$), a well-known result of collective variable theory [2,20]. The breather centered at a site is stable while the one centered at a bond is unstable [2];[1] its energy difference is the Peierls–Nabarro barrier. This energy difference acts as a barrier to mobile breathers for travelling along the lattice; the numerical computations of this barrier nicely fit with collective variable predictions.

Our main interest, however, focusses on mobile solutions, i.e., $p \neq 0$. How are Peierls–Nabarro barriers to mobility overcome by the fixed point solution? Our results show clearly that the uniquely continued p/q-resonant fixed point for $\nu \neq 0$ is spatially asymptotic to an *extended background*, whose amplitude increases from zero (at $\nu = 0$) with increasing nonintegrability ν, superposed to the moving (AL)-like core, see Fig. 1. In order to reveal the structure of this extended background, we have to pay attention to spatially extended solutions of the Salerno model.

The Salerno equation (2) admits extended solutions of the plane wave form, $\Phi_n(t) = A \exp[\mathrm{i}(kn - \omega t)]$, provided the following (nonlinear) dispersion relation holds:

$$\omega = -2\bigl[1 + (1 - \nu)|A|^2\bigr]\cos k - 2\nu|A|^2. \tag{8}$$

[1] That is the case for unstaggered ($\alpha = 0$)-continued stationary breathers from AL. The staggered breathers ($\alpha = \pi$) have its stability reversed, as shown in [2].

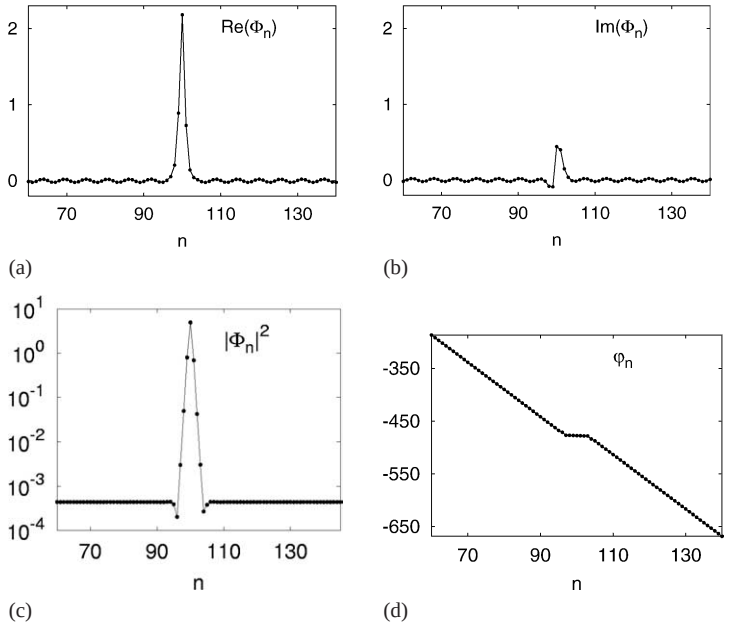

Fig. 1. Instantaneous profile of a 1/1 breather with $\omega_b = 4.909$ and $v_b = 0.7813$. Real part (a), imaginary part (b), modulus (c) and phase (d). The nonintegrability parameter in (2) is $\nu = 0.05$.

A p/q-resonant plane wave satisfies $\Phi_n(t) = \Phi_{n+p}(t + qT_b)$, and therefore, for a p/q-resonant plane wave the following condition also holds:

$$\frac{\omega}{\omega_b} = \frac{1}{q}\left(\frac{p}{2\pi}k - m\right), \tag{9}$$

m being any integer. Eqs. (8) and (9) can be solved for k and one obtains a finite number of branches $k_j(|A|)$ of p/q-resonant wave numbers in the first Brillouin zone, $-\pi \leqslant k_j \leqslant \pi$. The simplest case of a unique branch for fixed ν (as well as ω_b and p/q) and A small, is represented in (a) and (b) of Fig. 2. For example, for A small and $\omega_b > 4$, for any value of $0 < \nu < 1$ and A, there is a unique 1/1-resonant wavenumber branch $k_0(\nu, A)$.

For the general situation where several branches k_j ($j = 0, \ldots, s-1$) of resonant plane waves solve (8) and (9), the power spectrum of a background site n, $S(\omega) = |\int_{-\infty}^{\infty} \Re(\Phi_n(t)) \exp[\mathrm{i}\omega t]\, dt|^2$, reveals s peaks at the values ω_j corresponding to the resonant wave vector branches. The background is, up to numerical accuracy, a linear superposition of p/q-resonant plane waves, namely,

$$\sum_{j=0}^{s-1} A_j \exp\bigl[\mathrm{i}(k_j n - \omega_j t)\bigr].$$

The amplitudes A_j differ typically orders of magnitude, i.e., $|A_0| \gg |A_1| \gg |A_2| \gg \cdots$, so that only a few frequencies are dominant, for most practical purposes. One would speak of localization in k-space to describe the extended background of the p/q-resonant fixed point. Once the values of ω_b, v_b and ν are given, the "selection rule" provided by Eqs. (8) and (9), does not determine directly the resonant wave numbers k_j, but only branches $k_j(A)$. This reflects the inherent nonlinearity of the NLS lattice, where from the frequency of the plane wave depends on both wave number and amplitude in Eq. (8). Along the parametric continuation path the fixed point "adjusts" the plane wave content (k_j) of the background, so that it remains p/q-resonant under the changes in the amplitudes of the background plane waves (A_j).

4. Background relevance to mobility

Along the Newton continuation path to the standard DNLS equation the background amplitudes have a monotone increasing behavior with ν, see Fig. 3(a). High frequency solutions cannot be continued up to that limit, and the continuation stops for values of

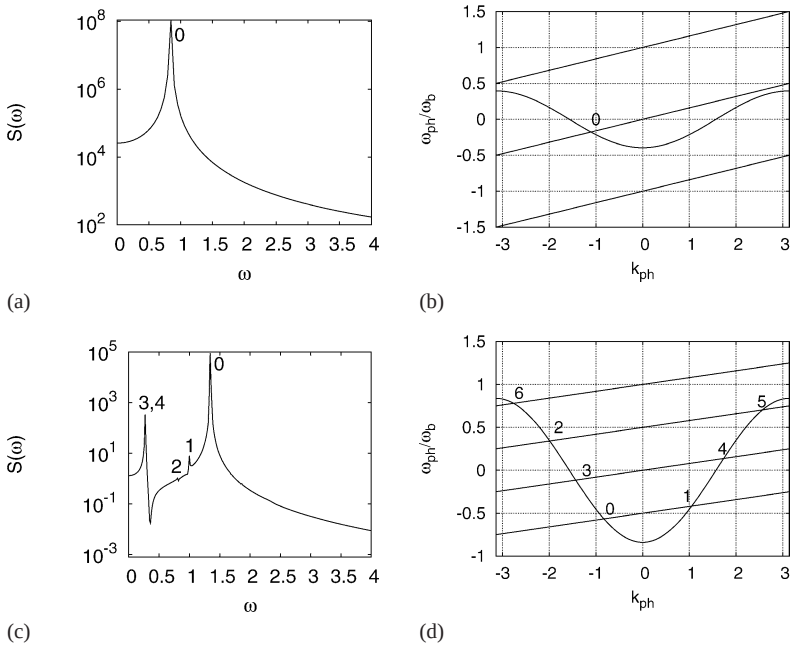

Fig. 2. Power spectrum. (a) $S(\omega)$ for the background of a $1/1$ breather with $\omega_b = 5.057$ at $\nu = 0.05$. In (b) formula (9) gives the contribution of a unique phonon ($j = 0$) with which agrees (Eq. (8)) with results given by $S(\omega)$. (c) $S(\omega)$ for the background of a $1/2$ breather with $\omega_b = 2.3842$ at $\nu = 1.00$. In (d) formula (9) gives the contribution of seven phonons ($j = 0, \ldots, 6$), but only five of them (0–4) are visible on $S(\omega)$. Note that the amplitudes $|A_j|$ differ by orders of magnitude.

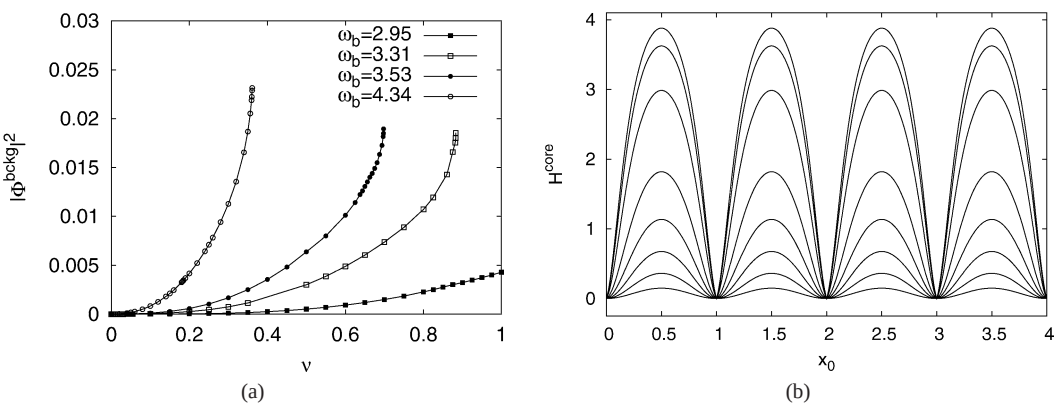

Fig. 3. (a) Background amplitude of different $1/1$ resonant breathers as a function of the nonintegrability ν. The amplitudes are zero in the AL integrable limit ($\nu = 0$) and have a monotone increasing behavior with ν. The value $\nu = 1$ corresponds to the standard DNLS equation. (b) Plot of H^{core} of a $1/1$ resonant breather with $\omega_b = 5.056$ as a function of the localization center x_0 for different values of ν (0.04, 0.08, 0.12, 0.16, 0.20, 0.24, 0.25 and 0.2512 (end of the continuation)). The amplitude of the oscillation of H^{core} grows with ν. (The minimum value of H^{core} has been set to zero in order to compare the differents functions.)

$\nu < 1$. This result correlates well with the collective variable (particle perspective) predictions [19,24] where the nonpersistence of travelling solutions is related to the growth of the Peierls–Nabarro barrier. In this respect, one observes a sudden increase in the background amplitude near the continuation border. This result reinforces the interpretation of the background as an energy support to the core for surpassing the (nonintegrable) Peierls–Nabarro barriers to mobility, and so its unavoidable presence for the exis-

tence of mobile breathers in the absence of integrability.

The role of the background in the localized core mobility can be analysed as follows. As the solution is unambiguously found to be $\hat{\Phi} = \hat{\Phi}^{\text{core}} + \hat{\Phi}^{\text{bckg}}$, the energy H, Eq. (5), of a mobile breather can be written as

$$H = H\left[\hat{\Phi}^{\text{core}}\right] + H\left[\hat{\Phi}^{\text{bckg}}\right] + H^{\text{int}}, \tag{10}$$

where H^{int} is the interaction energy, i.e., the crossed terms of $\hat{\Phi}^{\text{core}}$ and $\hat{\Phi}^{\text{bckg}}$ in the Hamiltonian. In the simplest case in which the background has a single resonant plane wave, its energy is a constant of motion (along with the total energy), so one obtains

$$\frac{\partial H[\hat{\Phi}^{\text{core}}]}{\partial t} = -\frac{\partial H^{\text{int}}}{\partial t}, \tag{11}$$

i.e., the variations of the core energy along the motion are balanced by the variations in the core–background interaction energy. Eq. (11) dictates the dynamics of any (eventual) effective (collective) variables intended to describe the mobile core in a particle-like description of the breather.

One can compute the core energy variations directly from the numerical integration of a solution by substracting (at each time step) the background from it. In Fig. 3(b) we plot the evolution of the core energy as a function of the core localization center, x_0, defined by using the norm N (Eq. (6)) of the Salerno model (2) as

$$x_0 = \frac{\sum_n n \ln(1 + \mu|\Phi_n^{\text{core}}|^2)}{\mu N}. \tag{12}$$

One observes that the core has extracted the maximum energy from the interaction term when the core passes over $x_0 = n \pm 1/2$ (maxima of the PN barrier) and has given it back to the interaction term at $x_0 = n$ (minima of the PN barrier). The bigger the PN barrier, the larger the interaction term (directly proportional to background amplitude) is. This result illustrate the role of the resonant background on the core mobility and the interpretation of its amplitude increase with ν. The increase of nonintegrability, and the subsequent growth of the PN barrier, demands additional support of energy from the interaction term, which is achieved by an increase of the background amplitude.

5. Conclusions

We have used a (SVD)-regularized Newton algorithm to continue mobile discrete breathers in the Salerno model from the integrable Ablowitz–Ladik limit. Our results indicate that, away from integrability, a description of these solutions based exclusively on localized (collective) variables is incomplete. The solutions are composed by a localized core and a linear superposition of plane waves, the background, whose amplitudes differ orders of magnitude. The background plays an important role in the translational motion of the localized core. Exact mobile localization only exist over finely tuned extended states of the nonlinear lattice. Mobile "pure" (i.e., zero background) localization must be regarded as very exceptional (integrability).

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