Multipulses in discrete Hamiltonian nonlinear systems

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In this work, the behavior of multipulses in discrete Hamiltonian nonlinear systems is investigated. The discrete nonlinear Schrödinger equation is used as the benchmark system for this study. A singular perturbation methodology as well as a variational approach are implemented in order to identify the dominant factors in the discrete problem. The results of the two methodologies are shown to coincide in assessing the interplay of discreteness and exponential tail-tail pulse interaction. They also allow one to understand why, contrary to what is believed for their continuum siblings, discrete systems can sustain (static) multipulse configurations, a conclusion that is subsequently verified by numerical experiment.

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In one spatial dimension, pulselike solutions are rather generic features of partial differential equations (PDE's) alongside kinks [1,2]. These are connections of a fixed point in phase space (representing a uniform steady state) with itself (in the case of a pulse) or with another fixed point (in the case of a kink). The above features present themselves in Hamiltonian [3] as well as in dissipative [4] systems. Typical applications on the parabolic side involve the propagation of stimuli down nerve axons in neurophysiology [5], the behavior of calcium release waves in living cells [6], the propagation of action potentials in the heart [7], or the concentrations of reactants in catalytic chemistry [8]. On the hyperbolic side also, however, applications abound: from the DNA double strand [9] to complex electronic materials [10] and from optical fibers to propagation of beams in waveguides [11,12]. It is, in particular, the latter class of models that we will deal with in this work. Furthermore, many of the applications mentioned above are, in their realistic implementation, not genuinely continuum but rather inherently discrete in nature. Hence, in this work we will study the behavior of pulses in such Hamiltonian nonlinear lattice models.

A simple generic system encompassing most of the phenomenological features of such problems is the discrete nonlinear Schrödinger (DNLS) equation. The DNLS was used by Jensen [13], Christodoulides, and Joseph [14] and later by Aceves *et al.* [15] to model the propagation of discrete self-trapped beams in arrays of coupled optical waveguides. It also serves as a generic envelope equation for discrete Klein-Gordon-type lattice equations; see, i.e., [9]. More recently, experimental work [16,17] has greatly increased the interest in such systems and has stimulated an intense theoretical effort to clarify the statics, dynamics, and thermodynamics of their pulselike patterns [18–22].

Most of these works were addressing the subject of single pulses and their stability. A problem that has been less adequately addressed, to the best of our knowledge, is the one of multipulses in such discrete Hamiltonian chains. Some first aspects of the problem were considered in [23] but were in part contradicted by the numerical findings of [24]. The multibreather technique when coming from the anticontinuum limit [25] can provide a number of useful results close to the $h\rightarrow\infty$ limit [24] (where h is the lattice spacing) but cannot be equally insightful when we consider cases close to the continuum and/or many lattice sites' comprising pulses as well as for configurations consisting of multiple copies of such coherent structures. It is interesting that in the continuum systems, some of these multipulse configurations have been proved to be unstable ([26] and references therein) and, in fact, all of them have been conjectured to be unstable in the same works.

Our purpose here is to show that, even if this is so for continuum systems, the statement is not true for discrete systems. Notably, we intend to show that there can exist stable stationary multipulse configurations in Hamiltonian nonlinear lattices. In showing that, we also intend to unify two seemingly different perspectives in addressing the problem. The first is the singular perturbation methodology formulated principally by Meron and co-workers (see, i.e., [27]) for continuum dissipative systems while the other is the variational approach adopted in [28]. The former method is adapted to the Hamiltonian and discrete setup and the results of the two are shown to coincide in extracting the prevalent contributing factors that balance each other in creating such stable structures. We finally support these claims by means of numerical evidence.

The DNLS equation reads

$$i\dot{u}_n=-\Delta_2 u_n-2|u_n|^2u_n, \tag{1}$$

where the overdot denotes time differentiation, n is the site index, u is the discrete complex field, and $\Delta_2 u_n=(u_{n+1}+u_{n-1}-2u_n)/h^2$. Now in accordance with [27], consider the *Ansatz*

$$u_n=\sum_{i=1}^{N} H_i(n;h,x_i)\exp(it), \tag{2}$$

where i indexes the pulses (which can be thought of as copies of an original pulse in a system with N pulses) and x_i indexes the "centers" of the pulses (when thought of as particles). Notice that, in essence, we now take the inverse viewpoint to the one of [24,25], seeking a qualitative and quantitative understanding of the relevant physical factors in the problem. H_i is a trial Ansatz for the form of the pulse. In particular, in NLS one can think of $H_i = p_i/\cosh(nh - x_i)$ (where $p_i = \pm 1$ is a parity variable). However, note, and we will return to this point, that the specific form of H_i will not be important for what follows. Also note that, per our Ansatz, we have implicitly rescaled the width of the solitary wave to 1 (or equivalently that we have rescaled all relevant length scales of the problem by dividing them by that width ρ^{-1}; hence our results can naturally be brought back to the case of $\rho \neq 1$ by the transformation $x_l \rightarrow x_l \rho$, where x_l is the length scale of interest). As per the non-exactness of the solution of Eq. (2), a correction factor $\epsilon R_n \exp(it)$ is used in the Ansatz, in the spirit of [27]. Also, to demonstrate the generality of the method, we exchange the nonlinearity $2|u_n|^2 u_n$ with a general nonlinear factor $\mathcal{N}(u_n)$ (which can permit, for instance, nonlinear gain-loss processes).

We now use that

$$\mathcal{N}\left(\sum_i H_i - \epsilon R_n\right) \approx \mathcal{N}\left(\sum_i H_i\right) - \epsilon \mathcal{N}'\left(\sum_i H_i\right) R_n \quad (3)$$

and the approximate identity (since the Ansatz for H_i will be close to the continuum form of the pulse)

$$-\sum_i H_i \approx -\Delta_2 \sum_i H_i - \sum \mathcal{N}(H_i). \quad (4)$$

Notice that the assumption is implicit in Eq. (4) that we are dealing with a "dilute gas" of pulses. This notion will be made more precise below [see point (iv) below on the stability of multipulses, as well as [27]]. Denoting by $\mathcal{L}$ the linearization operator

$$\mathcal{L} = i\partial_t - 1 + \Delta_2 + \mathcal{N}'\left(\sum_i H_i\right), \quad (5)$$

we use Eqs. (3)–(5) in substituting the Ansatz of Eq. (2) in Eq. (1). The equation can then be rewritten as

$$\epsilon \mathcal{L} R_n = \left[\mathcal{N}\left(\sum_i H_i\right) - \sum_i \mathcal{N}(H_i)\right]. \quad (6)$$

For reasons of simplicity, the dependence of the centers x_i on time is disallowed. This permits us also to automatically take care of the constraints (such as the conservation of the energy and of the norm of the solution) of the dynamical system of Eq. (1) and allows us to directly look for nonuniform effective steady states (since the H_i's will not depend on time) of the problem. For an overview as to why traveling (in the strict mathematical sense, defined, i.e., in Ref. [1]) may be problematic in discrete systems, the reader is referred to Ref. [29] and references therein. In fact, it was recently claimed in [30] that DNLS with local nonlinearity "does not admit moving breathers." For a generalized notion of traveling in systems of the type of Eq. (1), see, i.e., [31].

For a Hamiltonian system with N pulses, general theorems about the preservation of the number of eigenvalues will lead to the generation of N so-called translational mode pairs. These modes [32] correspond to translations of the pulses. In the continuum system, where translational invariance is a symmetry of the problem, the frequencies of such modes are 0. However, discreteness breaks translational invariance beyond all algebraic orders to cause an exponentially small bifurcation of the translational modes (i.e., their frequency becomes typically of $O\{\exp[-\pi^2/(2h)]\}$ [32,33]). We denote their respective eigenfunctions as p_k and we form the inner product of Eq. (6) with each of the bra vectors $\langle p_k|$. This is a classic method of obtaining collective coordinate equations, as is discussed in [34] (see also references therein). We thus obtain

$$\langle p_k|\mathcal{L}|R_n\rangle \approx \epsilon^{-1}\left\langle p_k \left| \sum_{i=1}^{N} \sum_{j\neq i} \mathcal{N}'(H_i) H_j \right.\right\rangle. \quad (7)$$

We now use the fact that $\langle p_k|$ is an eigenfunction of the operator $\mathcal{L}$ with eigenvalue ω, as well as the fact that $\langle p_k|$ is sharply peaked (and hence only linear terms in $H_{k\pm 1}$ will contribute to the expression; the more distant ones contribute higher-order terms in ϵ). We thus obtain

$$\omega\langle p_k|R_n\rangle = \epsilon^{-1}\langle p_k|F(H_k)(H_{k+1}+H_{k-1})\rangle, \quad (8)$$

where $F(H_k)$ is a suitable nonlinear function $[F(H_k) \approx \mathcal{N}'(H_k)$; see also Ref. [27]].

We now use the methodology of [27] *but for a Hamiltonian system*, where the eigenvalues will lie on the imaginary axis [under the conditions given below in point (iv)] and, hence, only the exponential term in the pulse interaction of the right-hand side (RHS) will survive [compare with Eq. (3.23) of [27]]. We also incorporate the results of [32,33] in which the asymptotics beyond all orders or the discrete Evans function methodologies have been used to provide a very accurate functional prediction for the translational mode frequencies. This result reads $\omega \approx C h^{-\beta} \exp[-\pi^2/(2h)]\sqrt{\cos(2\pi x_i/h)}$. The resulting final form of Eq. (8), which is the central analytical result of this work reads

$$C h^{-\beta} \exp\left(-\frac{\pi^2}{2h}\right)\sqrt{\cos\left(\frac{2\pi x_i}{h}\right)}$$
$$\approx a_0 \exp[-(x_{i+1}-x_i)] + a_1 \exp[-(x_i - x_{i-1})], \quad (9)$$

where a_0, a_1 are constants whose value will depend on the amplitude and parity of the pulses. Also, $x_{i+1} > x_i > x_{i-1}$ has been assumed (without loss of generality).

Some remarks are now in order. First, let us consider the case in which there are only two pulses. One can adopt a variational approach substituting in the DNLS Hamiltonian

$$H = \sum_n \frac{|u_{n+1}-u_n|^2}{2h^2} - |u_n|^4 \quad (10)$$

a two-pulse Ansatz $u_n = \Sigma_i p_i [1/\cosh(nh - x_i)]\exp(it)$. The ensuing Hamiltonian consists of the exponentially small (in the lattice spacing) terms of the Peierls-Nabarro barrier that is present due to discreteness for each pulse, as well as of the exponentially small tail interaction terms. This task was performed in [28]. Subsequent minimization of the Hamiltonian provides the equation for the equilibrium positions for the (multiple) potential equilibria of the pulses as

$$\frac{2\pi^5}{3h^4}\exp\left(-\frac{\pi^2}{h}\right)\sin\left(\frac{2\pi}{h}(x_i-x_j)\right)=\pm\exp(-2|x_i-x_j|) \tag{11}$$

and the center of mass $Z=(x_i+x_j)/2=0,h/2$ could be either centered on a site or centered between sites, respectively, for the plus or minus in Eq. (11). Now, if one considers Eq. (9), for each of the two pulses, the difference of the two equations will yield the "quantization" condition [$\sin(2\pi Z/h)=0$] on the center of mass, while the sum will result in an equation exactly like Eq. (11). As is highlighted in [28], stable multipulse configurations will result *independently* of whether $Z=0$ or $Z=h/2$, when these multipulses consist of two individually stable pulses. Unstable configurations will result from the concatenation of unstable individual pulses (again independently of the center-of-mass position), while saddle configurations will result from the concatenation of a stable and an unstable pulse. For more details, see Sec. III of Ref. [28]. The variational approach is quite useful in characterizing the two-pulse case but is rather cumbersome to apply for multipulses. On the other hand, the singular perturbation approach is more qualitative (the details of the constants depend, for instance, on the specifics of the eigenmodes) but captures very nicely the structure of the problem and the relevant physical factors contributing to it and can be easily generalized to an arbitrary number of pulses. However, we have shown that the two methods work in a consistent manner and lead to the following general conclusions regarding pulse trains.

(i) The generalization to multipulses. A lattice of pulses will form. If the individual constituent pulses are considered as "mesoscopic" particles [whose distance satisfies the criteria that will be set below; see point (iv)], then their mutual interaction (coupling) is Toda-like [the exponential term in their mutual separation resulting as in the RHS of Eq. (9)], but there is also a type of harmonic on-site substrate potential for each particle [the term coming from the translational eigenmodes in the LHS of Eq. (9)] whose amplitude is exponentially small in the lattice spacing, due to the Peierls-Nabarro (PN) barrier. The balance of these terms for N pulses [through the set of N Eqs. (9)] will give rise to a lattice of N pulses for any $N\geqslant 2$.

(ii) The continuum limit and the role of discreteness. The above description justifies why stationary continuum multipulses are so special and prone to instability. The exponential interaction in the absence of the balancing discreteness would necessitate motion of the pulse centers [27], unless a very special (possibly very symmetric) stationary configuration is achieved. These results also justify why discreteness has such ample possibilities for static multipulse configurations. The (periodic in the whole lattice) PN barrier creates a discreteness-induced force term that can balance the exponential (in the pulse distance) tail interaction.

(iii) Generality of conclusions. As mentioned before, on the one hand, this analysis has been performed for DNLS, which serves as a generic envelope equation in lattice Hamiltonian problems. Hence, at least within the appropriate time scales, the analysis will be applicable generically for Klein-Gordon-type equations also. Furthermore, notice that no specifics on the type of nonlinearity have been required. Furthermore, as has been shown for a variety of relevant models (see, i.e., [32,33]), the breaking of translational invariance due to discreteness leads to an exponential in h, harmonic in x_i behavior of the translational mode frequency ω similar to the one used above. This is also a general result, following from the Melnikov calculation of the splitting of homoclinic orbits in nonintegrable discrete systems [33]. Hence, the basic components of Eq. (11) are generic features of the systems of interest.

(iv) Stability of multipulses. The above results also show why stable multipulse configurations are possible in discrete systems. In particular, as has been remarked in [28], the full problem has translational modes close to the spectral origin. These modes "map" the curvature of the PN barrier. Suppose that all components of a multipulse solution are at corresponding local minima of the PN barrier. In that case, only interaction eigenmodes can be unstable. As was shown in [28], for two-pulse configurations when the pulses have opposite parity (up-down configuration), the (exponential in the pulse distance) interaction mode is stable. Hence, putting it in the language of [27], this $O(\epsilon)$ eigenvalue [where $\epsilon=\exp(-L)$, $L=|\Delta x_i|$] is stable. This conclusion naturally leads one to believe that only configurations of the form $\cdots$-up-down-up-$\cdots$ can be stable. As is shown by our analysis, such configurations will have an $O(\epsilon)$ contribution in their interaction modes from the up-down part and only a much weaker $O(\epsilon^2)$ effect from the up-up interaction (of next nearest neighbors). Consequently, such configurations should be stable. This conclusion was in fact verified by numerical experiments such as the one shown in Fig. 1. In this case, a Newton-Raphson numerical technique with appropriate selection of initial conditions was used to create an up-down-up configuration (on a 300-site lattice, with periodic boundary conditions and $h=0.5$) and subsequent numerical linear stability analysis confirms that the spectrum of this multipulse indicates stability. One may, however, worry that oscillatory instabilities resulting from the collision of the interaction eigenmodes with either the translational modes [35] or the continuous spectrum modes [22,35] might be possible (due to their opposite Krein sign [25,33]). Alas, the interaction eigenmodes behave as $\lambda\sim\exp(-L)$ while the translational eigenmodes behave as $\exp[-\pi^2/(2h)]$. For small and intermediate discreteness [up to $h\approx O(1)$] to ensure diluteness and stability against collisions of eigenvalues and oscillatory instabilities, one has a straightforward criterion by comparing the exponential dependences. Namely, if $L\gg\pi^2/(2h)$ [$L\gg\pi^2/(2h\rho^2)$ in dimensional units], then no such collisions will occur and the multipulse configurations will *not* suffer oscillatory instabilities. Notice that this condition is more stringent than the diluteness condition ($L\gg 1$; $L\gg 1/\rho$ in dimensional units). In most cases of small h, in fact, the condition may be overly conservative since the

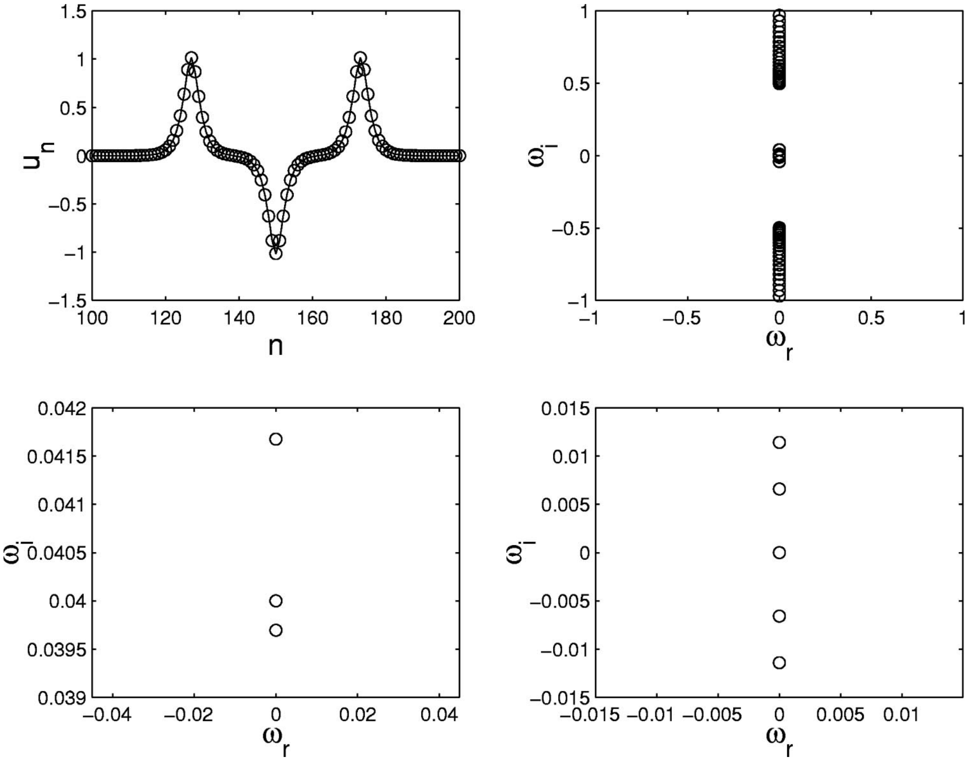

FIG. 1. A (stable) multipulse configuration and its spectrum. The top left subplot shows the spatial profile (the time-independent part of the solution) while the top right shows the spectral plane (ω_r, ω_i); the subscripts denote the real and imaginary part of the eigenvalues, respectively. The localized eigenmodes consist of three translational mode pairs of $|\omega| \approx 0.04$ (shown in the bottom left panel) and two interaction mode pairs of $|\omega| \approx 0.01$ as well as two remaining at zero (due to symmetry) eigenvalues (shown in the bottom right panel).

power-law prefactor ($h^{-\beta}$) of the translational eigenmodes will be important. For strong discreteness ($h \gg 1$), the translational eigenmodes have merged with the continuous spectrum (these eigenmodes do not have opposite Krein sign, at least not in the bright soliton case considered here). Hence, in this case, the oscillatory instability will appear due to collision of interaction eigenmodes with the continuous spectrum and a criterion for stability can be similarly derived by ensuring that $C \exp(-\rho L) \ll \Lambda$ [in dimensional units, with C a constant of $O(1)$ and Λ the solitary wave frequency]. Even though C is, in general, unknown, it can either be found very accurately by simulations (since the exponential dependence on the separation is very clear; see, i.e., [28]) or it can be approximated for a rough estimate by a constant of $O(1)$. In general, the more stringent one of the two (diluteness and stability) conditions can be enforced and then [i.e., if the pulse separation is larger than the critical one imposed by (the more stringent of) the two conditions], the multipulse configuration will *generically* be stable.

We believe that the above exposition clarifies the features relevant to multipulse problems in discrete systems. The exponentially small transversality effects of the orbits cause exponentially small (in the lattice spacing) eigenvalues [32], which can be evaluated very accurately via the approach of [32,33]. In turn, these effects give rise to a periodic, on the lattice, potential-energy barrier (of exponentially small amplitude) that consequently exerts a force on each pulse (a "substrate" force). Additionally, multipulse systems encompass the exponentially small (now in the interpulse distance) effects of tail interaction, which also cause an (attractive for the same parity, repulsive for opposite parity [28]) additional force. The balance of the two forces can be manifested both through the adjustment of singular perturbation theory to discrete Hamiltonian systems and/or the more popular (but less simple to generalize) variational approach in such systems. It can, in turn, lead to the generation of static multipulse configurations in such systems and a qualitative understanding both of such equilibria as well as of their potential stability. We have in fact shown explicitly numerically and justified analytically why such systems can, possibly contrary to their continuum siblings, support such stable multipulse entities. Notice the superiority of the singular perturbation technique developed herein with respect to the variational approach of [28], as it is unaffected (in its degree of complication) by the number of pulses involved and contains a clear physical intuitive explanation of the competing factors and the nature of the resulting equations. On the other hand, when it can be formulated, the variational method gives a more quantitative aspect of the problem. It should also be highlighted that on the basis of maintaining the diluteness of the gas of pulses studied herein and also of avoiding oscillatory instabilities (such as those explored in [35,22]), specific conditions for the pulse separation have been developed that allow one to state what is the critical pulse separation, beyond which, for *any* interpulse distance [satisfying Eq. (9)], such configurations will be stable. A possibly interesting generalization of these results could consist of a step similar to the one of paragraph 4.4 of [27], where a continuous (or possibly a genuinely discrete) medium of pulses is considered. Such "mesoscopic" lattices of pulses and of coherent structures more generally could be of relevance to many continuum as well as discrete systems. It should also be noted that in the case presented herein, the positions and amplitudes of the pulse centers were directly determined by the intrinsic dynamics of Eq. (1). However, should an appropriate external site-dependent potential be added, (stable) multipulses consisting of pulses of variable amplitude or of selected position can be achieved. For a detailed study of such phenomena, see, i.e., [36]. Finally, an interesting generalization of the work presented herein would involve more complicated *Ansätze* (than the one presented here), which could also account for variations of the height, width, and frequency of the nonlinear waves. Such challenging tasks will be left for future studies.

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