Appendix

A.1 Numerical Computation of Traveling Solitary Waves and Their Stability

A reasonable approximation to a genuine solitary wave solution of Eq. (1.3) can be obtained by simply imparting velocity to the first particle and simulating sufficiently long to let the solitary wave form [1]. A more accurate solitary wave can be obtained by a Newton iteration scheme. We summarize the discussion of [2] which details the procedure. First, we recall that genuine traveling waves of Eq. (1.6) with precompression satisfy the equation

$$\begin{aligned} 0 = &-c^2\phi_{\xi\xi} + \frac{A}{M}\{[\delta_0 + \phi(\xi - 1)]_+^p - 2\,[\delta_0 + \phi(\xi)]_+^p \\ &+ [\delta_0 + \phi(\xi + 1)]_+^p\}. \end{aligned} \tag{A.1}$$

where $\xi = n - ct$ and $\phi(\xi) = y_n(n - ct)$. To obtain numerical solutions of Eq. (A.1), we can employ a uniform spatial discretization of ξ consisting of L points ξ_k $(k = -\frac{L-1}{2}, \ldots, 0, \ldots, \frac{L-1}{2})$ with lattice spacing $\Delta\xi$ chosen such that $q = 1/\Delta\xi$ is an integer. Then, the field $\phi(\xi)$ is replaced by its discrete counterpart, i.e., $\phi_k := \phi(\xi_k) = \phi(k\Delta\xi)$. The second-order spatial derivative appearing in Eq. (A.1) is replaced by a modified central difference approximation $(\phi_{k-2} - 2\phi_k + \phi_{k+2})/(4\Delta\xi^2)$. The reason for this choice of central difference is connected to the stability calculation to be discussed below. Using this discretization, Eq. (A.1) becomes the following root-finding problem,

$$\begin{aligned} 0 = &-c^2\frac{\phi_{k-2} - 2\phi_k + \phi_{k+2}}{4\Delta\xi^2} + \frac{A}{M}\{\left[\delta_0 + \phi_{k-q}\right]_+^p \\ &- 2\,[\delta_0 + \phi_k]_+^p + \left[\delta_0 + \phi_{k+q}\right]_+^p\} \end{aligned} \tag{A.2}$$

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which can be solved via a Newton iteration scheme for the variables ϕ_k, see [3] for details on Newton iteration schemes. We employ periodic boundary conditions at the edges of the spatial grid. This method was employed to study solitary waves of the granular chain in [4] and rarefaction waves in lattices with strain-softening potentials (i.e., Eq. (1.3) with $p < 1$) [2], see also [5, 6] for other examples.

To investigate the spectral stability of a solution ϕ^0, we substitute the linearization ansatz $\Phi(\xi, t) = \phi^0 + \varepsilon a(\xi) e^{\lambda t}$ to arrive at Eq. (3.33), see Sect. 3.4. If ϕ^0 is localized in ξ, it can be seen as a compact perturbation of the eigenvalue problem in which $\phi^0 = 0$. Thus, we expect the continuous spectra of these eigenvalue problems to coincide [7]. If $\phi^0 = 0$, then we can solve Eq. (3.33) analytically with the ansatz $a(\xi) = e^{i\xi\ell}$, where the eigenvalues are given by

$$\lambda(\ell) = i\ell c \pm 2i \sin\left(\frac{\ell}{2}\right)\sqrt{\frac{pA\delta_0^{p-1}}{M}}. \tag{A.3}$$

This indicates that the continuous spectrum around the uniform steady state is purely on the imaginary axis. Thus, any instability of the wave will be due to point spectrum, which we must calculate numerically. We chose a discretization such that the spectra of the zero solution (see Eq. (A.3)) corresponds to the spectra of the zero solution of the discrete variant of Eq. (3.33). Using the standard central differences for the spatial derivatives appearing in (3.33) will lead to eigenvalues with a real part in the case of $\phi^0 = 0$. Hence, particular care needs to be taken to discretize the first and second derivative operators in a "compatible" way. Indeed, in order to avoid this "spurious instability," we used a modified central difference formula for the second spatial derivative, leading to the following eigenvalue problem

$$\lambda a_k = b_k, \tag{A.4}$$

$$\lambda b_k = -c^2 \frac{a_{k+2} - 2a_k + a_{k-2}}{4\Delta\xi^2} + c\frac{b_{k+1} - b_{k-1}}{\Delta\xi} + \tag{A.5}$$

$$p\frac{A}{M}\left\{\left[\delta_0 + \phi^0_{k-q}\right]_+^{p-1} a_{k-q} - 2\left[\delta_0 + \phi^0_k\right]_+^{p-1} a_k + \left[\delta_0 + \phi^0_{k+q}\right]_+^{p-1} a_{k+q}\right\}$$

which has been cast as a linear system in λ through the definition $a\lambda = b$ (such that standard eigenvalue solvers can be used), and where $a_k := a(k\Delta\xi)$. In the case of $\phi^0 = 0$, Eq. (A.4) with $k \in \mathbb{Z}$ is solved by $a_k = e^{ik\Delta\xi\ell}$, where the eigenvalues are given by

$$\lambda(\ell) = i\frac{\sin(\ell\Delta\xi)}{\Delta\xi}c \pm 2i \sin\left(\frac{\ell}{2}\right)\sqrt{\frac{pA\delta_0^{p-1}}{M}}, \tag{A.6}$$

which is consistent with Eq. (A.3) in the limit $\Delta\xi \to 0$ and perhaps even more importantly is also purely on the imaginary axis, suggesting neutral stability. While this choice of discretization seems reasonable, additional inconstancies may arise due to the finite nature of the computations and introduction of boundary conditions, which

are detailed in [2]. Thus, what the best discretization scheme is remains an open problem, although recent work suggests that spectral collocation schemes may be more well suited towards such a scope [8].

A.2 Numerical Computation of Breathers and Their Stability

We now provide a brief summary of how to compute time-periodic solutions in granular crystals (as well as more generally) and how to assess their stability by computing Floquet multiplers. We begin by writing Eq. (1.3) as a system of first order ODEs:

$$\dot{\mathbf{x}} = \mathbf{F}\left(t, \mathbf{u}, \mathbf{v}\right), \qquad \mathbf{x} = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \tag{A.7}$$

where $\mathbf{u} = \left(u_1, \ldots, u_p\right)^T$ and $\mathbf{v} = \dot{\mathbf{u}}$, respectively, represent the N-dimensional position and velocity vectors.

In order to find periodic solutions to this system, we are searching for solutions $\mathbf{x}$ so that $\mathbf{x}(0) = \mathbf{x}(T_b)$ where T_b is the fixed period of the solution. This suggests we define the Poincaré map: $\mathcal{P}(\mathbf{x}^{(0)}) = \mathbf{x}^{(0)} - \mathbf{x}(T_b)$, where $\mathbf{x}^{(0)}$ is the initial condition and $\mathbf{x}(T_b)$ is the result of integrating Eq. (A.7) forward in time until $t = T_b$ using standard ODE integrators [9]. A periodic solution with period T_b (frequency $1/T_b$) will be a root of $\mathcal{P}$. To obtain an approximation of this root, one can apply Newton's method to the map [10, Sect. 3],

$$\mathbf{x}^{(0,k+1)} = \mathbf{x}^{(0,k)} - \left[\mathcal{J}\right]^{-1}_{\mathbf{x}^{(0,k)}} \mathcal{P}\left(\mathbf{x}^{(0,k)}\right), \tag{A.8}$$

where k is the index of the Newton iteration and x^0 is the desired root of $\mathcal{P}$. The Jacobian of the map $\mathcal{P}$ is $\mathcal{J} = \mathbf{I} - V(T_b)$, where $\mathbf{I}$ is the $2N \times 2N$ identity matrix; V is the solution to the variational problem

$$\dot{V} = \left[\mathrm{D}F\right](t)\, V, \tag{A.9}$$

with initial data $V(0) = \mathbf{I}$; and $\mathrm{D}F$ is the Jacobian of the equations of motion Eq. (A.7) evaluated at the point $\mathbf{x}^{(0,k)}(t)$. For each step, one simultaneously solves Eq. (A.7) with initial data $\mathbf{x}^{(0,k)}$ and Eq. (A.9). This iteration scheme is applied until a user-prescribed tolerance criterion is satisfied. This method only ensures the solution is periodic in time, with period T_b, and does not, for example, yield necessarily a spatially localized structure. This highlights the importance of the initial step $\mathbf{x}^{(0,0)}$, which should have the desired spatial structure. The initial step (or guess) can be a linear mode or a solution to a continuum nonlinear approximation.

There is a rich theory for the stability properties of breathers in Hamiltonian systems, see [10, 4.2] and [11, 12]. A linear stability problem is determined in the

standard way: A small perturbation $V(t)$ is added to a solution $\mathbf{x}(t)$ that is time-periodic. The result $\mathbf{x}(t) + V(t)$ is substituted into Eq. (A.7) to obtain an equation describing the evolution of V. Keeping only linear terms in V will result in Eq. (A.9). Thus, using Newton iterations for computation of time-periodic solutions immediately yields stability information of that solution, as explained below.

Since $[\mathrm{D}F](t)$ will be periodic in time with period T_b, Eq. (A.9) represents a Hill's equation. It is well known within Floquet theory [13], that the fundamental solutions of Eq. (A.9) have the property $V(t + T_b) = \rho V(t)$, where ρ is a so-called Floquet multiplier (FM). The Floquet multipliers are the eigenvalues of the matrix $V(T_b)$, where $V(T_b)$ is the solution of Eq. (A.9) with initial data given by the identity matrix. Thus, the perturbation will exhibit exponential growth if there is at least one Floquet multiplier with $|\rho| > 1$. In this case, the corresponding solution $\mathbf{x}$ is deemed unstable. Otherwise, the solution is called spectrally stable. Due to the Hamiltonian structure of the system, all Floquet multipliers must lie on the unit circle for the solution to be spectrally stable, otherwise, the solution is unstable, see [10, Sect. 4] for more details. There are continuous arcs of spectrum on the unit circle (in the infinite-lattice limit), and one can compute these arcs from the linear spectral bands of Eq. (1.3). In general, the isolated multipliers (i.e., the "point spectrum") must be computed numerically. For Hamiltonian systems, there is always a pair of FMs at the point $+1$ (i.e., at the point $(1, 0)$ of the unit circle). These correspond to the invariance of the system under time translation—a feature responsible for the conservation of the total energy. By exploiting information about this FM pair, one can extract a stability criterion for breathers [14] that is reminiscent of the well-known Vakhitov–Kolokolov criterion for the stability of solitary waves, stating that when the monotonicity of the breather energy as a function of its frequency changes, its stability will change too. Equally remarkably, the fact that traveling waves are periodic orbits (modulo shifts) on the lattice has allowed to extend such a criterion to traveling waves in a criterion stating that when the monotonicity of the traveling wave energy as a function of its speed changes, then its stability should also change. This topic presently constitutes an active field of research [8].

Additional conservation laws of the system will lead to additional pairs of FMs at the point $+1$. Such FMs also complicate the computation of breathers using the Newton's method described above, since the Jacobian $\mathcal{J} = \mathbf{I} - V(T_b)$ is not invertible if there is a unit FM. To overcome this issue, one must break the degenerate nature of $\mathcal{J}$ by introducing additional constraints, such as a vanishing time average (i.e., $\int_0^T y_1(t)dt = 0$) or a pinning condition (e.g., $y_1(t) = 0$). In practice, it can also be effective to take a pseudoinverse of $\mathcal{J}$.

Finally, it is important to note that spectral stability does not exclude the possibility of algebraic growth of perturbations [15], or nonlinear instabilities [10]. For breathers in granular crystals, such cases have been checked through direct numerical simulations. See [10, 11] for numerous practical methods for computing the relevant periodic orbits and their stability.

A.3 Derivation of the Nonlinear Schrödinger Equation

The derivation of the nonlinear Schrödinger (NLS) equation from the granular chain model will follow a similar pattern as the derivation of the KdV equation that appears in Sect. 3.2. However, there is quite a bit of technical detail involved, even in the case of the monomer chain with precompression. The derivation of the NLS equation from a monomer FPUT lattice is given in [16], however not many details of the calculations are provided in that work. The derivation of the FPUT lattice with an onsite potential is considered in [17] (where also a rigorous justification is also provided), which is accompanied by a great level of detail. In [18], the NLS is derived in the strain variable formulation of the FPUT lattice. In [19], the NLS equation is derived from the strain variable formulation of the FPUT lattice in Fourier space and rigorously justified. The derivation presented here will be similar to [17], but will be modified since no onsite potential is present in granular chain.

We start the discussions from Eq. (1.3) in the case of the monomer, where all the prefactors A_n/M_n are equal. We write Eq. (1.3) in a slightly different form, which will make the notation for our derivation less cumbersome,

$$\frac{d^2u_n}{dt^2} = -V'(-\partial_n^+ u) + V'(-\partial_n^- u) \tag{A.10}$$

where the notation for the forward and backward differences are given by $\partial_n^+ = u_{n+1} - u_n$ and $\partial_n^- = u_n - u_{n-1}$, respectively. Here we have defined,

$$V'(x) = \frac{A[\delta_0 + x]^p}{M}$$

which has absorbed the mass M. Assuming now that the relative displacements satisfy

$$u_{n-1} - u_n \ll \delta_0 \tag{A.11}$$

we can approximate $-V'(-x)$ with its third order Taylor polynomial,

$$\begin{aligned} -V'(-x) \approx W'(x) = J_1 + J_2 x + J_3 x^2 + J_4 x^3, \qquad J_1 = \frac{A\delta_0^p}{M} \\ J_2 = \frac{Ap\delta_0^{p-1}}{M}, \quad J_3 = -\frac{Ap(p-1)\delta_0^{p-2}}{2M}, \quad J_4 = \frac{Ap(p-1)(p-2)\delta_0^{p-3}}{6M} \end{aligned} \tag{A.12}$$

Note that J_s is defined simply as $J_s = K_s/M$ for $s = 1...3$. We use this notation to avoid dividing by M throughout the derivation. Recognizing that the leading terms vanish when using the approximation $W'(x)$ instead of $-V'(-x)$ in Eq. (A.10), we can see that our new model acquires the form of an FPUT lattice [20] according to:

$$\frac{d^2u_n}{dt^2} = W'(\partial_n^+ u) - W'(\partial_n^- u) \tag{A.13}$$

Note, we defined $W'(x)$ through the Taylor expansion of $-V'(-x)$ rather than $V'(x)$ in order to obtain an FPUT model in the standard form shown in Eq. (A.13). The remainder of the analysis will be on Eq. (A.13).

The linear part of Eq. (A.13) (namely when $J_3 = J_4 = 0$) has the form

$$\frac{d^2u}{dt^2} = Lu = J_2(\partial_n^+ u - \partial_n^- u) \tag{A.14}$$

and was analyzed in Sect. 1.2. It was shown that the linearized equation has plane wave solutions

$$E_n(t) = e^{i(kn+\omega(k)t)}$$

where $\omega(k)$ is given by the dispersion relation,

$$\omega(k)^2 = 2J_2(1 - \cos(k)).$$

We will study the modulation of planes waves under the evolution of the nonlinear equation Eq. (A.13) using the ansatz

$$u_n(t) = \epsilon U(X, T)E_n(t) + \text{c.c} + \text{h.o.t.} \qquad X = \epsilon(n - ct), \quad T = \epsilon^2 t \tag{A.15}$$

where c.c. is the complex conjugate and h.o.t are higher order terms (see below). This choice may appear to be somewhat unexpected at first, however, it is possible to convince ourselves that it is the most natural one. We scale space by ϵ, in which case the dispersive scaling of NLS' space and time derivatives necessitates that we use an ϵ^2 for the time rescaling. As regards the ansatz of the solution, we seek a solution that explicitly includes a breathing in time (with frequency $\omega(k)$) and a spatial modulation with wavenumber k. The motivation here is that we have in mind a rapidly oscillating plane wave that is modulated by a slow envelope provided by $U(X, T)$. The factor of ϵ for the amplitude ensures that the solution is of small amplitude, making the Taylor expansion used previously valid. Direct substitution of ansatz (A.15) into Eq. (A.13) will generate higher order harmonics (i.e., terms like E^s) and thus one must include an ansatz incorporating all possible harmonics. Thus, we will work with the ansatz,

$$u_n(t) \approx \psi_n(t) = \sum_{s=1}^{3} \epsilon^s \sum_{j=-s}^{s} U_{s,j}(X, T)E_n(t)^j \tag{A.16}$$

where $U_{s,j} \in \mathbb{C}$ and $U_{s,-j} = \overline{U_{s,j}}$. Note, this implies $U_{s,0} \in \mathbb{R}$ for $s = 1, 2, 3$. Inserting this ansatz into Eq. (A.13) will produce a fairly large expression. To manage this,

we will collect terms according to the power in ϵ, but also their power in E to create a hierarchy of solvability conditions. Moreover, within each of these orders, we will organize terms in three different parts, namely those coming from the left-hand side of Eq. (A.13) (the time derivative part), the linear part $L\psi$, and the nonlinear part $N(\psi)$, which is defined as,

$$N(\psi) = J_3[(\partial_n^+\psi)^2 - (\partial_n^-\psi)^2] + J_4[(\partial_n^+\psi)^3 - (\partial_n^-\psi)^3]$$

As we will see below, the NLS equation appears at the order $\epsilon^3 E$. This explains why we only include powers up to $s = 3$ in our ansatz. The forward and backward differences of the ansatz have the form

$$\partial_n^{\pm}\psi_n = \pm \sum_{s=1}^{3} \epsilon^s \sum_{j=-s}^{s} \left(U_{s,j}(X \pm \epsilon)e^{\pm ikj} - U_{s,j}(X)\right) E^j$$

where we have dropped the subscript and arguments of $E_n(t)$ and the T argument from $U_{s,j}(X, T)$ for notational simplicity. Rather than substituting this expression directly into the right-hand side of Eq. (A.13), we make use of the expansion

$$U(X \pm \epsilon) = U(X) \pm \partial_X U(X)\epsilon + \partial_X^2 U(X)\frac{\epsilon^2}{2} + \mathcal{O}(\epsilon^3) \tag{A.17}$$

Note that since the lowest order term in our ansatz has order ϵ, we need not keep the $\mathcal{O}(\epsilon^3)$ terms in the expansion given in Eq. (A.17). This is because the solvability conditions at $\mathcal{O}(\epsilon^4)$ will not be needed to derive the NLS equation. Below, we list the solvability conditions appearing at each order. All terms appearing on the left-hand side of the equality will be those resulting from the time derivative part $\frac{d^2\psi}{dt^2}$. All terms appearing on the right-hand side of the equality without an underline will be those resulting from the linear term $L\psi$. Finally, all terms appearing on the right-hand side of the equality with an underline will be those resulting from the nonlinear part $N(\psi)$.

We start with the $\mathcal{O}(\epsilon)$ terms, in which there is only one solvability condition:

$$\epsilon^1 E^1 : \qquad -\omega^2 U_{1,1} = -2J_2(1 - \cos(k))U_{1,1}$$

This equation is satisfied if ω obeys the linear dispersion relation $\omega^2 = -2J_2(1 - \cos(k))$. Moving on to the $\mathcal{O}(\epsilon^2)$ terms, we have two solvability conditions:

$$\begin{aligned} \epsilon^2 E^1 : &\qquad -\omega^2 U_{2,1} - 2i\omega c\partial_X U_{1,1} = -\omega^2 U_{2,1} + 2i\omega\omega'\partial_X U_{1,1} \\ \epsilon^2 E^2 : &\qquad -4\omega^2 U_{2,2} = -\omega^2(2k)U_{2,2} - \underline{J_3 s_1 c_1 U_{1,1}^2} \end{aligned}$$

Here we used the fact that $\omega^2 = 2J_2(1-\cos(k))$ and $\omega\omega' = J_2\sin(k)$. Later, we will also use the fact $(\omega')^2 + \omega\omega'' = J_2\cos(k)$. The definitions $s_1 = 2i\sin(k)$ and $c_1 = 2(1-\cos(k))$ also simplify the relevant expressions. The equation for $\epsilon^2 E^1$ yields the group velocity relation: $c = -\omega'(k)$. The equation for $\epsilon^2 E^2$ yields an expression for $U_{2,2}$

$$U_{2,2} = \frac{J_3 s_1 c_1}{4\omega^2 - \omega^2(2k)} U_{1,1}^2 \tag{A.18}$$

Note that $4\omega^2 \neq \omega^2(2k)$ for $k \neq 0$. Finally, moving on to the $\mathcal{O}(\epsilon^3)$ terms, we have the solvability conditions:

$$\begin{aligned}
\epsilon^3 E^0: \quad & c^2\partial_X^2 U_{1,0} = (\omega'(0))^2\partial_X^2 U_{1,0} + 2J_3 c_1(\overline{U_{1,1}}\partial_X U_{1,1} + U_{1,1}\partial_X\overline{U_{1,1}}) \\
\epsilon^3 E^1: \quad & -\omega^2 U_{3,1} - 2i\omega c\partial_X U_{2,1} + c^2\partial_X^2 U_{1,1} + 2i\omega\partial_T U_{1,1} \\
& = -\omega^2 U_{3,1} + 2i\omega\omega'\partial_X U_{2,1} + [(\omega')^2 + \omega\omega'']\partial_X^2 U_{1,1} \\
& \underline{+2J_3 s_1 c_1\overline{U_{1,1}}U_{2,2} - 2J_3 c_1\partial_X U_{1,0}U_{1,1} - 3J_4 c_1^2|U_{1,1}|^2 U_{1,1}} \\
\epsilon^3 E^2: \quad & -4\omega^2 U_{3,2} - 4i\omega c U_{2,2} \\
& = -\omega^2(2k)U_{3,2} + 2i\omega(2k)\omega'(2k)\partial_X U_{2,2} \\
& \underline{+2J_3 c_1(c_1-3)U_{1,1}\partial_X U_{1,1} - 2J_3 s_1 c_1 U_{1,1}U_{2,1}} \\
\epsilon^3 E^3: \quad & -9\omega^2 U_{3,3} = -\omega^2(3k)U_{3,3} \\
& \underline{+2J_3 s_1(c_1 + s_1^2)U_{1,1}U_{2,1} + J_4 c_1^2(3-c_1)U_{1,1}^3}
\end{aligned}$$

The equation for $\epsilon^3 E^0$ yields,

$$\partial_X^2 U_{1,0} = \frac{2J_3 c_1}{c^2 - (\omega'(0))^2}\partial_X|U_{1,1}|^2$$

Integrating both sides, and setting the integration constant to zero, yields

$$\partial_X U_{1,0} = \frac{2J_3 c_1}{c^2 - (\omega'(0))^2}|U_{1,1}|^2 \tag{A.19}$$

Using Eqs. (A.18) and (A.19), and the fact that $c = -\omega'(k)$, the equation for $\epsilon^3 E^1$ simplifies to

$$2i\omega\partial_T U_{1,1} = \omega\omega''\partial_X^2 U_{1,1} + \left[2\frac{(J_3 s_1 c_1)^2}{4\omega^2 - \omega^2(2k)} - \frac{(2J_3 c_1)^2}{c^2 - (\omega'(0))^2} - 3J_4 c_1^2\right]|U_{1,1}|^2 U_{1,1} \tag{A.20}$$

Simplifying once more, we arrive at the NLS equation:

$$i\partial_T U_{1,1} = \frac{\omega''}{2}\partial_X^2 U_{1,1} + \frac{c_1^2}{2\omega}\left[2\frac{(J_3 s_1)^2}{4\omega^2 - \omega^2(2k)} - \frac{(2J_3)^2}{c^2 - (\omega'(0))^2} - 3J_4\right]|U_{1,1}|^2 U_{1,1} \tag{A.21}$$

The functions $U_{3,2}$ and $U_{3,3}$ can be calculated from $U_{1,1}$ using the equations for $\epsilon^3 E^2$ and $\epsilon^3 E^3$ respectively. If one wants to express the solution in the strain variable $y_n = \partial_n^+ u$, we simply compute the forward difference of our ansatz. To first order, this is

$$y_n = \partial_n^+ \psi = \epsilon(U_{1,0}(X+\epsilon) - U_{1,0}) + \epsilon\left[(U_{1,1}(X+\epsilon)e^{ik} - U_{1,1})E + c.c.\right] + \mathcal{O}(\epsilon^2)$$

Using once again the expansion Eq. (A.17) the approximation in the strain becomes

$$\partial_n^+ \psi = \epsilon(U_{1,1}(e^{ik} - 1)E + c.c.) + \mathcal{O}(\epsilon^2)$$

Note, the terms without the harmonic factors, $U_{1,0}$ have vanished. Now, we define an envelope function for the strain $Y(X,T) = U_{1,1}(X,T)(e^{ik} - 1)$, such that our ansatz for the strain equation becomes (up to first order)

$$y_n(t) = \epsilon Y(X,T)E + \text{c.c.}$$

If we substitute $U_{1,1} = Y(X,T)(e^{ik} - 1)^{-1}$ into Eq. (A.21) and simply, we obtain,

$$i\partial_T Y - \frac{\omega''}{2}\partial_X^2 Y - \frac{c_1}{2\omega}\left[2\frac{(J_3 s_1)^2}{4\omega^2 - \omega^2(2k)} - \frac{(2J_3)^2}{c^2 - (\omega'(0))^2} - 3J_4\right]|Y|^2 Y = 0 \tag{A.22}$$

where we used the fact that $|e^{ik} - 1|^2 = c_1$. Note, this is the same as the NLS equation in the displacement formulation, except for the fact that the nonlinear coefficient is scaled by the factor c_1 (compare Eqs. (A.21) and (A.22)). If we let $k = \pi$, then we have $s_1 = 0$, $c = 0$, $c_1 = 4$ and so the nonlinear coefficient

$$\nu_3 = -\frac{c_1}{2\omega}\left[2\frac{(J_3 s_1)^2}{4\omega^2 - \omega^2(2k)} - \frac{(2J_3)^2}{c^2 - (\omega'(0))^2} - 3J_4\right]$$

reduces to

$$B = \frac{1}{J_2\sqrt{J_2}}(3J_4 J_2 - 4J_3^2)$$

where we used the fact that $(\omega'(0))^2 = J_2$ and $\omega(\pi) = 2\sqrt{J_2}$. This is the value of the nonlinear coefficient of the NLS equation appearing in Sect. 4.1.

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