Localized versus traveling waves in infinite anharmonic lattices

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Abstract

Localized and traveling modes are worked out for an infinite anharmonic atomic chain by implementing a shooting algorithm and the finite difference and Newton procedures, respectively. These methods unlike the other currently used ones yield exact solutions in simulations carried out by integrating the equation of motion under the relevant initial conditions. © 2002 Elsevier Science B.V. All rights reserved.
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1. Introduction

Anharmonicity is known to condition energy localization or equipartition [1,2] and structural changes [3, 4] in periodic crystals, including biomolecules such as DNA [5,6]. Intrinsic localized excitations called breathers [7] and traveling waves which are the counterpart of the phonons typical of harmonic lattices, are instrumental in this process. Breathers were investigated for various lattice dynamical models by using mainly expansion based schemes such as the rotating wave approximation (RWA) [8,9] or the quasi-discreteness approach [10] and the uncoupled oscillator limit (UOL) [11]. In RWA the vibrational field associated with the breather is looked for as an exponentially damped sine-wave whereas in UOL it is obtained by switching on continuously [12] a harmonic, interatomic coupling within a finite coding sequence of anharmonic, initially uncoupled oscillators. Simulations carried out by solving the equations of motion in large crystals with initial conditions inferred from RWA or UOL always produce vibrational fields decaying in the long term into phonon-like oscillating tails named as nanopteron [7]. This general behavior has been interpreted as signalling an instability but it results actually from a generic shortcoming due either to the approximate nature of RWA or to finite size effects in UOL. Alternatively the stability of breathers has been analyzed within the linear Floquet approximation [7,11, 13], which may contradict the conclusions derived by simulation.
By contrast with breathers very little is known on time-periodic traveling waves in anharmonic lattices. Their existence has been ascertained only in the integrable model of Toda [14] for the cnoidal waves where a Floquet analysis [15] has concluded on their stability. Anharmonic phonons have also been studied numerically in infinite [16] Fermi–Pasta–Ulam and Lennard–Jones lattices where they proved to be unstable within a Floquet analysis. UOL has been extended to a finite sequence of phase-shifted breathers [2,17] to mimic traveling anharmonic phonons, which gave rise to nanopertons for the same reason as mentioned above for breathers. Likewise since the calculated properties of breathers and traveling modes depend in UOL upon the chosen coding sequence, no conclusive evidence of their existence could be brought about from a comparison with experiment [18].

In this Letter the properties of breathers and oscillatory traveling waves, including displacement patterns-amplitude-dependent vibrational frequencies and dispersion curves, will be presented for infinite crystals. This difficulty could be overcome thanks to the very knowledge of the asymptotic behavior and the implementation of the relevant boundary conditions for breathers and traveling waves, respectively. The localized excitations have been worked out by extending the shooting procedure [19] to asymmetric potentials whereas the traveling ones have been achieved by combining the finite difference and Newton methods [16,20,21]. Both numerical procedures yield exact vibrational patterns, free from nanopertons and stable under simulations so that localized and traveling excitations remain indefinitely decoupled without undergoing any deformation. The Toda and Fermi–Pasta–Ulam (FPU) potentials, chosen for illustration, have an acoustic branch, which will turn out to condition strongly the properties of both localized and traveling modes. The FPU model was introduced [22] to assess the role of anharmonicity in energy relaxation [23] in solids. Toda’s model [14] is one of the few integrable lattice cases [24] and we have used the corresponding cnoidal waves to check the validity of our calculational scheme. As shown for solitons [20], the full system of nonlinear equations proves to decouple into one-particle equations, thus providing an exact quasi-particle picture for the motion of breathers and some traveling waves.

Let us consider an infinite chain of oscillators of mass unity, coupled by the potential

$$V = \sum_{i \in \mathbb{Z}} W(u_i - u_{i+1}),$$

where \(u_i\) designates the displacement coordinate of the particle \(i\) with respect to its static equilibrium position. As the pair potential \(W(x_i)\) is assumed to be a function of the difference \(x_i = u_i - u_{i+1}\), there are infinitely many equilibrium configurations, all characterized by equidistant atoms. We are concerned with Toda’s model \(W_1\) and the FPU potential \(W_2\),

$$W_1 = e^x, \quad W_2 = \frac{x^2}{2} + \frac{\lambda x^3}{3} + \frac{x^4}{4},$$

where \(\lambda \in \mathbb{R}\) is taken as a disposable parameter. The equations of motion at time \(t\) read

$$\ddot{u}_i(t) = \frac{dW}{dx}(x_{i-1}) - \frac{dW}{dx}(x_i), \quad i \in \mathbb{Z}. \quad (1)$$

2. Breathers

A breather-like solution of Eqs. (1) comprises the infinite sequence \(\{u_{i\in\mathbb{Z}}(t)\}\), characterized by

$$u_i(t + T) = u_i(t),$$

$$u_{i \to \pm \infty}(t) \to u_{\pm \infty}, \quad \forall i, \quad (2)$$

where \(T\) is the vibrational period and \(u_{\pm \infty} \in \mathbb{R}\) refer to the asymptotic limits. Due to the Toda and FPU models having a harmonic limit, the vibrational field decays exponentially [19] at infinite distances,

$$\left\{u_{i \to \pm \infty}(t) - u_{\pm \infty}\right\} \propto e^{\pm \lambda} \sin(\omega t),$$

$$\omega^2 = 2 - r - r^{-1}, \quad (3)$$

where \(|r| < 1\) and \(\omega = 2\pi/T\) is the vibrational frequency. The Toda and FPU models have the same phonon dispersion \(\omega_p(k) = \omega_M \sin(k/2)\), where \(\omega_p\) and \(k \in [0, \pi]\) stand for the phonon frequency and wave vector, respectively, and \(\omega_M = 2\) is the largest phonon frequency. It ensues that \(\omega > \omega_M\) and hence \(\omega > \omega_p(k), \forall k\). Thus the breather and phonon frequencies cannot be degenerate in an infinite crystal because the phonon field extends up to infinite distances by contrast with the spatially localized one of a breather. Note that UOL leads to the opposite conclusion that...
phonons can arise inside the phonon band as phonobreathers [11,25].

All velocities \( \dot{u}_i \) are assumed to vanish simultaneously, consistent with the time-behavior of \( u_{i-}\to\pm\infty(t) \) in Eqs. (3). Then as neither \( t \) nor \( \dot{u}_i \) appear explicitly in Eqs. (1), it comes \( u_i(t) = u_i(T/2 - t) \) since \( \dot{u}_i(T/4) \) has been taken to vanish. Therefore it suffices to confine oneself to the range \( t \in [-T/4, T/4] \) and the solution of Eqs. (1) depends on a single parameter \( \omega \). In an infinite lattice, vibrational patterns such that \( u_i(t) = -u_{i-1}(t) \) for odd \([11,25]\) and even, are consistent with Eqs. (1) for any pair potential being a function of \( u_i = -u_{i+1} \). The analysis will be illustrated on the odd case and only outlined for the even one. In the odd case, Eqs. (1) are to be solved for \( i = -n, \ldots, n \) and \( t \in [0, T/4] \) under the boundary conditions

\[
\begin{align*}
  u_0(0) &= 0, & u_{i>0}(0) &= -u_{i-1}(0), \\
  \dot{u}_{i>0}(0) &= \dot{u}_{i-1}(0), & \dot{u}_i \left( \frac{T}{4} \right) &= 0,
\end{align*}
\]

\[
\frac{u_{i+1}(t) - u_{i-1}(t)}{u_{i+1}(t) - u_{i-1}(t)} = r(\omega),
\]

where \( r(\omega) \) is given by Eqs. (3) and \( n \) is taken large enough so that \( |u_{i+1}(t) - u_{i-1}(t)| \approx 1, \forall t \) (as explained below, \( n = 4 \) proved to fulfil that condition).

As Toda’s model sustains no breathers, we turn to the FPU potential \( W_2 \) with \( \lambda = 1 \). A shooting procedure [19] has first been implemented for \( \lambda = 0 \), in which case the unknowns reduce to the initial velocities \( \{\dot{u}_{i=0,\ldots,n}(0)\} \). Advantage has been taken of

\[
\frac{u_{i+1}(t) - u_{i-1}(t)}{u_{i+1}(t) - u_{i-1}(t)} \approx \frac{\dot{u}_{i+1}(0)}{\dot{u}_{i-1}(0)}
\]

so that the system of differential equations in (1) is turned into one of ordinary equations solved to get accurate estimates of the initial velocities. The latter are used subsequently to integrate Eqs. (1). Then the \( \lambda = 0 \) initial velocities are used as starting values to integrate repeatedly Eqs. (1) at \( \lambda \neq 0 \) for the unknowns \( \{u_{i=1,\ldots,n}(0), \dot{u}_{i=0,\ldots,n}(0)\} \), while increasing \( \lambda \) stepwise up to \( \lambda = 1 \) and taking the step size small enough to keep the convergence fast, i.e., till we get \( |u_{i=1,\ldots,n}(T/4)| < 10^{-14} \) for each \( \lambda \) value. The computed \( u_i(t) \)’s are plotted in Fig. 1. The data display the fast decay \( u_i(\to t) \to u_{\pm\infty}(\omega) = \pm 0.514, \forall t \), because of \( |r| \ll 1 \) \( (r(\omega = 4) = -0.072) \). The \( \omega \) dependence of the vibrational amplitude on site \( i \), defined as \( a_i = |u_i(T/4) - u_i(0)| \), is depicted in Fig. 2. As expected from Eqs. (3), the breather and phonon frequencies are checked not to be degenerate since the breather displacement field vanishes allover the phonon frequency range \([0, \omega_M]\). Every \( a_i \) starts growing from 0 at \( \omega = \omega_M \) with an infinite slope and decreases with \( i \) like \( |r|^i \) at fixed \( \omega \) and \( i > 1 \). Whereas \( a_i(\omega) \) keep increasing with \( \omega \), every
$a_{i > 4}(\omega)$ eventually vanishes because of $r \propto \omega^{-2}$ for $\omega \gg \omega_M$ as follows from Eqs. (3) so that $a_{i=4}(\omega) \ll 1$, $\forall \omega$, thereby justifying our assumption made in Eqs. (4) that the harmonic regime has indeed set in for $i > 4$ and $u_{i > 4}(t)$ is hence accurately given by Eqs. (3).

As the breathers are time-periodic and the shooting method consists of integrating exactly Eqs. (1) over $T$ with an accuracy better than $10^{-14}$, the breathers are recognized to be stable in a simulation performed over an arbitrarily large time $NT$ ($N \gg 1$), unlike those computed by RWA [8] or UOL [11, 13]. Likewise even and odd breathers proved [27] to be stable or not, respectively, within a Floquet analysis whereas both turn out to be stable in our simulations.

The analysis proceeds along the same line in the even case $u_i(t) = -u_{i-1}(t)$. Eqs. (1) have been solved over $t \in [-T/4, T/4]$ for the unknowns $\{u_i(0), \dot{u}_i(0)\}$ under the conditions

\[
\begin{align*}
  u_{-1}(0) &= -u_0(0), \\
  \frac{u_{n+1}(t) - u_\infty}{u_n(t) - u_\infty} &= r(\omega).
\end{align*}
\]

The displacements $u_i(t)$ and the vibrational amplitudes, defined as $a_i = |u_i(T/4) - u_i(-T/4)|$, are plotted in Figs. 3 and 4, respectively. They call for the same comments as Figs. 1 and 2.

As $\dot{u}_i(t)$ does not vanish for $t \in [0, T/4]$ (see Fig. 1), the set of site-shift operators $\{g_i(x)\}$ such that $u_{i+1}(t) = g_i(u_i(t))$ can be inverted to give $u_i(t) = g_i^{-1}(u_{i+1}(t))$. Eqs. (1) are recast into

\[
\begin{align*}
  \ddot{u}_i &= h_i(u_i), \\
  h_i(x) &= \frac{dW}{dz}(g_{i-1}^{-1}(x) - x) - \frac{dW}{dz}(x - g_i(x)).
\end{align*}
\]

A time-conserved energy per site $\varepsilon_i$ can be defined owing to the kinetic energy theorem:

\[
\varepsilon_i = \frac{\dot{u}_i(0)^2}{2} = \frac{\dot{u}_i(t)^2}{2} - \int_{u_i(0)}^{u_{i+1}(t)} h_i(x) \, dx. \quad (5)
\]

Because a time-invariant energy $\varepsilon_i$ can be ascribed to each atomic degree of freedom $u_i$, the first-order differential system in Eqs. (5), wherein the $\varepsilon_i$’s come in as parameters, and the second-order differential system in Eqs. (1) are equivalent. Furthermore, the total breather energy $\varepsilon$ reads as a sum of one-body energies $\varepsilon_i$:

\[
\varepsilon = \sum_{i \in \mathbb{Z}} \varepsilon_i, \quad \varepsilon_i = \varepsilon_i + W(u_i(0) - u_{i+1}(0)). \quad (6)
\]

Moreover, the full many-body Hamiltonian $H$, whence Eqs. (1) originate, decouples exactly in a sum of one-body Hamiltonians $H = \sum_{i \in \mathbb{Z}} H_i$, similarly to the
case of solitons [20,21]:
\[ H_i = \frac{u_i^2}{2} + \tilde{W}_i(u_i), \quad \tilde{W}_i(u_i) = - \int_{u_i(0)}^{u_i(t)} h_i(x) \, dx. \]

Each anharmonic Hamiltonian \( H_i \) is to be compared with its harmonic counterpart \( H_k \),
\[ H_k = \frac{q_k^2}{2} + \omega_k^2(k) \frac{q_k^2}{2}, \quad q_k = \sum_{j=1}^{N} e^{iku_j}, \]
where \( q_k \) is the phonon normal coordinate associated with the wave-vector \( k \) and \( N \) refers to the crystal size.

3. Traveling waves

A traveling wave of vibrational period \( T \) and phase velocity \( \tau^{-1} \) (the lattice parameter is set equal to 1) is characterized in an infinite crystal by
\[ u_{i+1}(t) = u_i(t), \quad u_i+1(t) = u_i(t + \tau), \quad \forall t. \tag{7} \]
The wave length \( l \), wave vector \( k \) and frequency \( \omega \) fulfill \( l = T/\tau \) and \( kl = \omega l = 2\pi \), which results in \( k = \omega \tau \). Because of \( \tau \leq T \), it comes \( k \in [0, 2\pi] \), which assigns the size of the one-dimensional Brillouin zone.

Eqs. (1) are recast into
\[ \ddot{u}(t) = \frac{dW}{dx}[u(\tau - t) - u(t)] - \frac{dW}{dx}[u(t) - u(t + \tau)]. \tag{8} \]
A solution \( u(t) \) of Eq. (8), obeying Eqs. (7) in an infinite crystal, can be sought such that \( u(t) = -u(\tau - t) \) because this is consistent with every pair potential function of \( u_i - u_{i+1} \). This implies that \( \langle u_i \rangle = (1/T) \int_0^T u_i(t) \, dt = 0 \), i.e., the time-averaged displacement coincides with the static equilibrium position so that traveling waves cannot induce static distortion by contrast with breathers [8]. It suffices to consider the range \( t \in [0, T/2] \) and it comes \( u(0) = u(T/2) = 0 \). Moreover, \( u(t) \) and \( -u(t) \) are both solutions if \( W(x) = W(-x) \).

A similar rationale consisting of replacing \( u(t), \tau \) by \(-u(t), \tau \) in Eq. (8) leads to the conclusion that to each solution \( u(t) \), with given \( T, \tau \), there corresponds the solution \(-u(t)\) associated with \( T, -\tau \). Consequently, the wave-field \( \{\pm u_i(t)\} \) may as well propagate in two opposite directions associated with respective phase velocities \( \pm \tau^{-1} \). Accordingly the relationship \( \omega(k) = \omega(-k) \), valid for phonons, holds also for anharmonic modes whence \( k \) can be confined within the range \([0, \pi]\).

A solution \( u(t) \) of Eq. (8) is looked for, under the requirement that \( \ddot{u}(t) \) vanish a single time at \( t_M \in [0, T/2] \) and the vibrational amplitude is taken to be \( a = u(t_M) \). In case of \( W_1 \), Eq. (8) is to be solved under the conditions
\[ t \in [0, t_W = T/2], \quad u(0) = u(T/2) = 0, \]
\[ u(t < 0) = -u(-t), \quad u(t > T/2) = -u(T - t). \tag{9} \]
If \( W(x) = W(-x) \), as is the case for \( W_2 \) with \( \lambda = 0 \), the solution \( u(t) \) has additional properties. As Eq. (8) is symmetric with respect to interchanging \( u(t - \tau) \) and \( u(t + \tau) \), integrating it from \( t = t_M \) with \( \ddot{u}(t_M) = 0 \) yields \( u(t) = u(2t_M - t) \) and hence \( u(2t_M) = u(0) = 0 \). Moreover, consistency with \( u(t) = -u(-t) = -u(4t_M - t) = -u(T - t) \) requires to set \( t_M = T/4 \) and \( a = u(t_M) \). Finally, in case of \( W_2 \) with \( \lambda = 0 \), Eq. (8) will be integrated for
\[ t \in [0, t_W = T/4], \quad u(0) = 0, \]
\[ u(t < 0) = -u(-t), \quad u(t > T/4) = u(T - t). \tag{10} \]

The nonlinear differential equation in Eq. (8), having \( u(t) \) as the single unknown and including advanced \([u(t + \tau)]\) and retarded \([u(t - \tau)]\) terms, has been solved by combining the finite difference and Newton methods. The time range \([0, t_W]\) is first discretized, so that Eq. (8) turns into a system of finite difference equations for the unknown vector \( \bar{U} \) having \( n \) components \( U_{j=1,...,n} \):
\[ U_{j-1} + U_{j+1} - 2U_j \theta^2 = f(U_{j-m}, U_j, U_{j+m}). \tag{11} \]
The time duration \( \theta \ll 1 \) and the integers \( m, n \) are related by \( m\theta = \tau, n\theta = t_W \) and \( U_j = u(j\theta) \). Eqs. (11) are solved by Newton’s method, enforcing the boundary conditions of Eqs. (9) and (10) in the \( n \times n \) Jacobian matrix at \( t = 0, t_W \). The solution \( u(t) \) is found to depend on two parameters, namely the amplitude \( a \) and the wave-vector \( k \). Eqs. (11) have been first solved at the edge of the Brillouin zone \( k = \pi \) because Eq. (8) reduces there to an ordinary differential equation thanks to \( u(t \pm \tau) = -u(t) \). Likewise it proves
convenient to assume \( u(t) = \alpha \sin(\omega t) \) as a starting assignment for \( U \), \( \alpha \) being an estimated vibrational amplitude. Afterwards \( k \) is decreased stepwise by \( \delta k \) down to 0 by taking, prior to each iteration, the previously obtained \( u(t) \) as a starting assignment of \( U \). The convergence of Newton’s method has been considered to be achieved provided Eqs. (11) are satisfied within an accuracy better than \( 10^{-10} \). This result could be secured readily by taking \( \delta k = 0.05 \).

The displacement patterns \( u(t) \) and dispersion curves \( \omega(k) \) have been calculated over the whole Brillouin zone for \( W_1, W_2 \) and \( \lambda = 0 \) and plotted in Figs. 5 and 6. For sizeable \( a \), \( u(t) \) looks like a sine-wave (as for phonons) for \( k \gtrsim \pi/2 \), whereas for \( k \approx 0 \) it is more resemblant of either a sawtooth or a square wave for \( W_1 \) or \( W_2 \), respectively. The same conclusion has been reached by other authors [16]. At fixed \( k \) the amplitude \( a \) decreases with decreasing \( \omega \) and vanishes for \( \omega \) reaching its minimum value equal to the acoustic phonon frequency \( \omega_\phi(k) \). The dispersion curves associated with \( W_1 \) in Fig. 6 agree with those of cnoidal waves [14] provided appropriate boundary conditions are taken into account, which confirms the validity of our computation and supports the conclusion that our solutions are identical to those found analytically by Toda. The harmonic regime is retrieved for \( a \ll 1 \) so that \( u(t) \approx a \sin(\omega_\phi(k)t), \forall k \in [0, \pi] \).

Owing to \( \dot{u}(t) \in [0, T/4] \) \( \neq 0 \) in case \( W_1(x) = W_2(-x) \), the mapping \( t \mapsto u \) can be inverted to define the time-shift operators \( g_{\pm}(u) \) so that \( u(t \pm \tau) = g_{\pm}(u(t)) \). Eq. (8) is rewritten as

\[
\ddot{u} = h(u), \quad h(u) = \frac{dW}{dx}(g_-(u) - u) - \frac{dW}{dx}(u - g_+(u)). \tag{12}
\]

Applying the kinetic energy theorem to Eq. (12) permits to introduce the time-conserved energy per site

\[
\varepsilon = \frac{u(0)^2}{2} = \frac{\dot{u}(t)^2}{2} - \int_0^t h(y) \, dy, \tag{13}
\]

which is independent of site \( i \). Provided the potential \( W(x) \) is even, the many-body motion, described by Eq. (8) which includes the coupled coordinates \( u_1, u_{1\pm 1} \), is exactly accounted for by Eq. (13) involving a single unknown \( u(t) \) and the invariant \( \varepsilon \) as a parameter. By contrast, because Toda’s potential \( W_1(x) \) is not even, \( \dot{u}(t) \) vanishes for \( t \in [0, tw] \), as seen in Fig. 5, which prevents us from defining \( g_{\pm}(u) \) and thence \( \varepsilon \). However, Toda’s model is integrable [14], which means that there is one invariant per degree of freedom \( u_1 \), in particular for every cnoidal wave, but it is emphasized that none of them can be given the meaning of a one-body energy. Meanwhile Toda’s soliton [20] displays such a one-body decoupling.

In order to assess to which extent the \( \theta \)-dependent patterns \( u(t) \), computed for \( W_1, W_2 \) by solving
Eqs. (11), are accurate solutions of Eq. (8), we perform two kinds of simulations. First we integrate iteratively over $[0,T_F]$, 
\[
\ddot{v}_j(t) = \frac{dW}{dx}(v_{j-1}(t - \tau) - v_j(t)) \\
- \frac{dW}{dx}(v_j(t) - v_{j-1}(t + \tau)),
\]
for the sequence of unknown functions $\{v_j(t)\}$ taking as initial conditions $v_j(0) = v_{j-1}(0), v_j(0) = \dot{v}_{j-1}(0)$. The iteration is started for $v_1(t)$, taking $v_0(t) = u(t)$. Note that Eq. (14) is an ordinary differential equation with respect to the unknown $v_j(t)$ since the previously determined $v_{j-1}(t)$ plays the role of a known parameter field. As the iteration number $j$ grows towards its final value $j_f \gg 1$, thus mimicking a propagation over a large crystal comprising $j_f$ of unit-cells, the sequence $v_j(t)$ is found to converge towards $u(t)$ as far as the error $\max_{t \in [0,T_F]}|u_j(t) - u(t)|$ remains $< 10^{-6}$ for every $j = 1, \ldots, j_f$.

Then we solve Eqs. (1) for $i = 1, \ldots, 64$ over $[0,T_f \gg T]$ under initial conditions $\{u_i(0), \dot{u}_i(0)\}$ set by $u(t) \rightarrow u_i(0) = u(i \tau), \dot{u}_i(0) = \dot{u}(i \tau)$, assuming $u_1(t) = u_{64}(t)$. Wt. As the sequence $\{u_1, \ldots, u_{64}\}$ is found to obey Eqs. (7) with an accuracy better than $10^{-12}$, we conclude that anharmonic phonons are stable in both kinds of simulation despite the disturbance due to rounding errors and the finite size of the time step used in the numerical integrations.

4. Conclusion

Displacement patterns and vibrational frequencies have been worked out in infinite anharmonic one-dimensional lattices for breathers and traveling waves. Whereas the equations of motion decouple exactly into one-body equations for every breather and there is a time-invariant energy $\epsilon_i$ per degree of freedom, traveling waves exhibit the same properties only if the pair potential is even. Breather and phonon frequencies cannot be degenerate. However, even though localized and traveling waves happen to have the same frequency, they still remain decoupled because their different respective behaviors at infinite distance $u_i(t) \rightarrow \pm\infty(t)$ cancel any mutual coupling. By contrast with RWA and UOL results which always show up unstable in simulations, breathers and traveling modes obtained in this work prove to be exact and stable solutions of Eqs. (1), (8) as far as they fulfill Eqs. (2), (7), respectively, over arbitrarily large time durations. As a by-product they provide conclusive, numerical evidence for the existence of such modes and are thence prone to a comparison with experimental results.

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References

[26] Actually, the assumption made in Ref. [8] $\phi_i = \phi_{-i}$ for the odd case is inconsistent with $u_i(t) = -u_{-i}(t)$ and Eqs. (1) too (it should read $\phi_i = -\phi_{-i}$).