Phonon Scattering by Breathers  
in the Discrete Nonlinear Schrödinger Equation

Sungsik Lee*, Julian J.-L. Ting† and Seunghwan Kim‡  
Department of Physics, Pohang University of Science and Technology, San 31 Hyojadong, Pohang, Korea 790-784  
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Linear theory for phonon scattering by discrete breathers in the discrete nonlinear Schrödinger equation using the transfer matrix approach is presented. Transmission and reflection coefficients are obtained as a function of the wave vector of the input phonon. The occurrence of a nonzero transmission, which in fact becomes perfect for a symmetric breather, is shown to be connected with localized eigenmodes thresholds. In the weak-coupling limit, perfect reflection are shown to exist, which requires two scattering channels. A necessary condition for a system to have a perfect reflection is also considered in a general context.

I. INTRODUCTION

Breathers, which also called oscillating solitons, are time periodic and spatially localized excitations ubiquitously found on translationally invariant coupled nonlinear lattice [1-3]. It was introduced first in the context of the sine-Gordon equation in 1974 [4]. It requires practically no activation energy and thus bridge the gap between the highly nonlinear modes and the linear phonon modes. Such long-lived spatially localized excitation has fundamental significance in the dynamics of spatially extended systems. It has been found that the discreteness of a system plays an essential role on the stability of breathers in several systems [5]. It introduces a cut-off frequency to the system so that the resonance between the phonon band and the frequency of the discrete breather can be avoided.

However, breathers grow and decay due to their interaction with the environment. Some of such interactions which has been studied include the electron-breather interaction [6] and the interaction of breathers with extended defect [7]. The discrete breather can play a role of the scattering center affecting energy transport by scattering, absorbing or radiating phonons. Since the phonon is a major form of radiations for small amplitude excitations in the nonlinear lattice, it is important to characterize such breather-phonon interaction [8].

Recently it has been found that scattering properties of the breather are related to the structure of the internal modes of the breather itself [9]. They studied the phonon scattering by a kink in the localized equilibria of the nearest neighbor interacting chain and showed that the scattering properties undergo a drastic change, involving a perfect transmission, as the localized eigenmode threshold is passed. It was conjectured that this result on the static localized structure could be extended to a wide class of systems with time-dependent localized structures such as breathers. It has also been confirmed in the case of time periodic discrete breather in the Hamiltonian nearest neighbor chain both numerically and using the extended Levinson theorem [8].

The purpose of this paper is to present the analysis of phonon scattering by breathers in the discrete nonlinear Schrödinger (DNLS) equation using the transfer matrix method. We proved analytically that at the localized eigenmode threshold the transmission at the phonon band edge, such that the wave vector \( k = 0 \), is nonzero, which in fact becomes perfect in the case of symmetric breather. This result is also confirmed by numerical calculations with transfer matrices. The crucial difference of the DNLS equation from the localized equilibria of the nearest neighbour chain is that it allows two scattering channels [9]. This

*Electronic address: ssong@anyon.postech.ac.kr  
†Electronic address: jting@anyon.postech.ac.kr  
‡Electronic address: swan@postech.ac.kr
allows occurrence of the perfect reflection whose existence is shown in detail in the weak-coupling limit. A necessary condition for a system to have a perfect reflection is obtained in comparison with the case of the local equilibria in the classical Hamiltonian systems. We end with discussions on extensions of our results to more general systems including the time-periodic discrete breathers in the Hamiltonian chain.

II. THE TRANSFER MATRIX FORMULATION

There are many ways to discretize the nonlinear Schrödinger equation. One of the widely studied version, called the DNLS equation, reads,

\[ \dot{\psi}_n = i \left( |\psi_n|^2 \psi_n + \epsilon (\psi_{n-1} + \psi_{n+1}) \right), \]

in which \( \psi_n \) is the amplitude at site \( n \) and \( \epsilon \) is the coupling strength. If one consider a solution of the form \( \psi_n = a_n e^{i\omega t} \) for Eq. (1), \( a_n \)'s satisfy

\[ \omega a_n = a_n^3 + \epsilon (a_{n-1} + a_{n+1}). \]

Without loss of generality, we could choose \( \omega > 0 \). We further consider only the 1-site breather, i.e. only one site is excited on the lattice. Hence for zero-coupling the breather solution centered at the origin is given by

\[ \psi_n = a_n e^{i\omega t} \]

in which

\[ a_n = \sqrt{\omega} \]

The linearization of Eq. (2) around the breather solution with \( \phi_n = \psi_n - a_n e^{i\omega t} \) yields,

\[ \dot{\phi}_n = i \left( 2a_n^2 \phi_n + a_n^2 e^{i2\omega t} \phi_n^* + \epsilon (\phi_{n+1} + \phi_{n-1}) \right). \]

Because of the complex conjugate operation on \( \phi_n \), at least two frequency components are necessary for the solution of Eq. (3). Therefore, the DNLS equation can allow two scattering channels different from the case of localized equilibria with a single scattering channel [3]. If we assume \( \phi_n = b_n e^{i(\omega + \Omega) t} + c_n e^{i(\omega - \Omega) t} \), with \( b_n \) and \( c_n \) complex, we obtained the following equations:

\[ \begin{pmatrix} \omega + \Omega - 2a_n^2 & 0 \\ 0 & \omega - \Omega - 2a_n^2 \end{pmatrix} \begin{pmatrix} b_n \\ c_n \end{pmatrix} = \epsilon \begin{pmatrix} b_{n-1} + b_{n+1} \\ c_{n-1} + c_{n+1} \end{pmatrix}. \]

With \( Y^T_n = (b_n, c_n, b_n^*, c_n^*) \), the above equation can be written in a recursive form as

\[ \begin{pmatrix} Y_n \\ Y_{n-1} \end{pmatrix} = M_n \begin{pmatrix} Y_{n+1} \\ Y_n \end{pmatrix}, \]

in which \( M_n \) is a function of \( a_n, \epsilon, \omega \) and \( \Omega \). The matrix \( M_n \) is called a transfer matrix, which maps a pair of linearized coordinates on one site to another site [4]. Applying Eq. (5) successively from the site \( N \) to the site \( -N \), one has

\[ \begin{pmatrix} Y_{-N} \\ Y_{-N-1} \end{pmatrix} = M \begin{pmatrix} Y_{N+1} \\ Y_N \end{pmatrix}, \]

with \( M = M_{-N} \cdot M_{-N+1} \cdots M_{N-1} \cdot M_N \).

Far from the center of the breather, \( a_n \) decays to zero, so that Eq. (6) becomes decoupled, with solutions of the form \( b_n = e^{ik_n n} \) and \( c_n = e^{ik_n n} \), in which \( \cos k_n = (\omega + \Omega) / 2\epsilon \) and \( \cos k_n = (\omega - \Omega) / 2\epsilon \). The solutions of \( b_n \) and \( c_n \) define two possible scattering channels. Each channel can be either a traveling (phonon) mode with a real wave vector \( k \) or an exponentially growing (decaying) mode with an imaginary \( k \) depending upon the values of \( |\omega \pm \Omega| / 2\epsilon \). Since \( \epsilon \) and \( \Omega \) occurs only in the form of ratios \( \epsilon / \omega \) and \( \Omega / \omega \), we can set \( \omega = 1 \) and regard \( \epsilon \) and \( \Omega \) as dimensionless variables. The boundaries of the phonon bands are given by \( \omega = \Omega \pm 2\epsilon \) and \( -\Omega \pm 2\epsilon \). These phonon bands divided the parameter space of \( \epsilon \) and \( \Omega \) into three regions according to the number of traveling channels as shown in Fig. [4].
III. THE SCATTERING PROBLEM

In a Levison theorem, the bound state property of a system is related to its scattering property \([12]\). In what follows, the property of scattering in region-1 was related to the property of localized mode in region-0.

Firstly, we consider the scattering problem in region-1. In the standard scattering setup, a phonon is incident with normalized amplitude from the left side of the breather located at the origin. We assume \(\Omega > 0\). The case with \(\Omega < 0\) can be handled similarly.

The question asked in a scattering problem is its transmission and reflection coefficients. It can be shown from the DNLS equation that

\[
Im \langle \psi^\mu_{n+1} \psi_n \rangle = Im \langle \psi^\mu_{n} \psi_{n-1} \rangle ,
\]

in which \(\langle A \rangle\) is the time average of \(A\). This flux-conservation relation makes the one-channel scattering process elastic, i.e.,

\[
|t|^2 + |r|^2 = 1,
\]

in which \(t\) and \(r\) are transmission and reflection coefficients respectively.

Suppose the channel \(c_n\) is a traveling mode with \(k_c\) real, while \(k_b = i\kappa_b (\kappa_b > 0)\) is imaginary. The asymptotic solutions are of the form

\[
\begin{align*}
    b_n &= b_i^n e^{\kappa_b n} \\
    c_n &= e^{i k_c n} + c_i^n e^{-i k_c n} & \text{if } n \to -\infty, \\
    b_n &= b_r^n e^{-\kappa_b n} \\
    c_n &= c_r^n e^{i k_c n} & \text{if } n \to \infty,
\end{align*}
\]

in which the amplitude of the incident phonon on the channel \(c_n\) is set to unity. The amplitudes for the transmitted and reflected phonons, \(c_r^n\) and \(c_i^n\), fully characterize the one-channel phonon scattering by a symmetric breather. Since Eq.(8) is not covariant under multiplication of an arbitrary phase factor \(e^{i\theta}\) on \(b_n\) and \(c_n\), it may appear that the scattering properties depend on the phase of the input phonon. However, if \(b_n\) and \(c_n\) are solutions of Eq.(8), so are \(ib_n\) and \(-ic_n\). Therefore, transmission and reflection are independent of the phase of the input phonon in the one-channel scattering case.

Inserting Eq.(8) into Eq.(5), we obtain 8 linear equations with 8 variables to solve for, i.e.

\[
\begin{pmatrix}
    b_1^n e^{-\kappa_b N} \\
    e^{-ik_c N} + c_i^n e^{ik_c N} \\
    b_i^n e^{-\kappa_b N} \\
    e^{i k_c(N+1)} + c_i^n e^{-i k_c(N+1)} \\
    b_r^n e^{-\kappa_b(N+1)} \\
    e^{-ik_c(N+1)} + c_i^n e^{ik_c(N+1)} \\
    b_1^n e^{-\kappa_b(N+1)} \\
    e^{i k_c(N+1)} + c_i^n e^{-i k_c(N+1)}
\end{pmatrix}
= M
\begin{pmatrix}
    b_i^n e^{-\kappa_b(N+1)} \\
    c_i^n e^{ik_c(N+1)} \\
    b_i^n e^{-\kappa_b(N+1)} \\
    c_i^n e^{-i k_c(N+1)} \\
    b_r^n e^{-\kappa_b(N+1)} \\
    e^{i k_c(N+1)} + c_i^n e^{-i k_c(N+1)} \\
    b_1^n e^{-\kappa_b(N+1)} \\
    e^{-ik_c(N+1)} + c_i^n e^{ik_c(N+1)}
\end{pmatrix}.
\]

For \(k_c = 0, 1 + c_i^n\) can be treated as one complex variable. The resulting 8 homogeneous equations have a non-trivial solution only on their null space.

On the other hand, if both channels are non-traveling modes with both \(k_b = i\kappa_b (\kappa_b > 0)\) and \(k_c = i\kappa_c (\kappa_c > 0)\) imaginary. After discarding all exponentially growing parts, the asymptotic solutions read,

\[
\begin{align*}
    b_n &= b_i^n e^{\kappa_b n} & \text{if } n \to -\infty, \\
    c_n &= c_i^n e^{-\kappa_c n} \\
    b_n &= b_r^n e^{-\kappa_b n} & \text{if } n \to \infty, \\
    c_n &= c_r^n e^{-\kappa_c n}
\end{align*}
\]

The localized eigenmode is given by a solution of
of Eq.(6), \( \vec{Y} \) represents the traveling phonon in the scattering process. If the incoming phonons from the left side of the breather generate outgoing phonons, because they affect only the phase factors in the order \( \epsilon/\omega \). Therefore, the existence of additional channels with exponentially decaying parts is essential for a perfect reflection. Hence, there is no perfect reflection in two-channel phonon scattering. This provides a necessary condition for a linear system to allow a perfect reflection.

Our derivation does not depend on the specific form of the transfer matrix \( M \). The result is entirely based on the fact that asymptotic solutions which are composed of traveling phonon parts and exponentially growing or decaying parts far from the center of the breather can be connected to each other by a transfer matrix. Therefore, the same procedure can be applied to the breather-phonon scattering problem in the nearest neighbor Hamiltonian chain to obtain a similar proof [8]. A major difference is that the number of channels in the latter case should be extended to infinity for each frequency component \( \Omega + \omega_b \), in which \( \Omega \) is the phonon frequency and \( \omega_b \) is the breather frequency, in the case of Hamiltonian breather.

IV. PERTURBATIVE AND NUMERICAL CALCULATIONS

The occurrence of the perfect reflection in the weak-coupling limit can be shown by a perturbation method. Retaining only terms of order \( \epsilon/\omega \), we obtain the transfer matrix \( M \approx M_{-1} \cdot M_0 \cdot M_1 \); other \( M_n \)'s are discarded because they affect only the phase factors in the order \( \epsilon/\omega \). The transmission coefficient thus obtained is
The breather becomes opaque to the fourth power of the coupling strength. A perfect reflection occurs at $k_c = \pi/2$ in the weak-coupling limit. Numerical calculation, which takes into account of several higher order terms of $\epsilon/\omega$, agrees with the perturbative result as shown in Fig.\ref{fig:fig3}. Perfect phonon reflection by breathers in the DNLS equation is a property which persists for weak-coupling, in contrast to what happens in the Hamiltonian nearest neighbor chain where the perfect reflection exist only for a positive interval of coupling strength $\epsilon$ for a given $\omega_b$.

In the case of phonon scattering by a local equilibria kink in the nearest neighbor Hamiltonian chain, there is no perfect reflection \cite{8}. However, there occurs a perfect reflection in the Hamiltonian discrete breather \cite{6}. The critical difference between the case of a local equilibria kink and the case of Hamiltonian or the DNLS breathers is the minimum number of frequencies needed for describing linearized motion at each site. In the case of the local equilibria, one Fourier component measuring the deviation from the equilibrium at each site is sufficient to describe the motion of each site because the kink in the local equilibria is a time independent defect. On the other hand, the discrete breather in the Hamiltonian system has an intrinsic time scale $T_b$ which is the period of the breather. The intrinsic frequency $\omega_b = 2\pi/T_b$ generates an infinite number of frequencies $\Omega + m\omega_b$ ($m$ is an integer ) mixing with the phonon frequency $\Omega$ by nonlinear terms in the equation. For the DNLS case, only one more frequency is generated due to the complex conjugate operation in Eq.\ref{eq:10}.

With the transfer matrix method, the transmission and reflection coefficients can be calculated numerically in the same way as in the case of the local equilibria \cite{8}. The transfer matrix, $M$, is obtained numerically and the scattering coefficients are solved from Eq.\ref{eq:10}. The number of sites in the scattering setup, $N$, in Eq.\ref{eq:10} is chosen to allow a decay of the amplitude of the breather within the error bound, $10^{-2}$, in our calculation. For $0.01 < \epsilon < 0.4$, $N$ needs not to exceed 5 to maintain this bound.

The phase diagram for the localized eigenmodes and the transmission for various values of $\epsilon$ are obtained numerically in Fig.\ref{fig:fig4} and Fig.\ref{fig:fig5}. For small coupling, there is no perfect transmission. A perfect transmission is generated from $k_c = 0$ at $\epsilon = 0.262$ where a symmetric localized eigenmode \cite{13} is generated from the lower edge of the phonon band. The value of $k_c$ where the perfect transmission occurs increases from zero until it reaches a maximum value. Then the maximal wave vector decreases and becomes zero again where another localized eigenmode, which is anti-symmetric at this time \cite{13}, is generated. These numerical results are consistent with predictions of the linear scattering analysis.

The return of $k_c$, where the perfect transmission occurs, to zero after its initial creation and deviation from zero is due to the multi-site spreading of the breather envelope. For a one-site breather, if only $M_0$ is retained in calculating $M$, the location of the perfect transmission does not return to $k_c = 0$ again; which is consistent with the fact that there is no generation of the anti-symmetric localized eigenmode. In other words, the generation of a perfect transmission and a symmetric localized eigenmode is due to the single-site defect property of the discrete breather, whereas the annihilation of the perfect transmission and the generation of an anti-symmetric localized eigenmode is due to the multi-site structure of the breather.

The perfect reflection at nonzero $k_c$ is another special feature of the one-channel phonon scattering case. It is important because the breather can be regarded as a perfect reflecting barrier for the phonon, which opens the possibility of trapping phonons between two breathers. Numerical results show that a perfect reflection occurs at a special value of $k_c$ if the coupling is not too strong. The value of $k_c$ where the perfect reflection occurs changes from $\pi/2$ to 0 as $\epsilon$ increases. If $\epsilon$ reaches a critical value of 0.36, the perfect reflection disappears through $k_c = 0$ as depicted in Fig.\ref{fig:fig5}.

\begin{equation}
|t|^2 = 2(\epsilon/\omega)^4 \sin^2 2k_c.
\end{equation}

V. CONCLUSION

In conclusion, phonon scattering by discrete breathers in the DNLS equation is formulated by the transfer matrix method and transmissions were obtained in the one-channel scattering case. The nonzero transmission of phonons through the discrete breather at $k = 0$ in the one-channel phonon scattering occurs at the localized eigenmode threshold is proven analytically to be perfect for the symmetric discrete breather. Numerically, the perfect transmission was shown to occur at $k = 0$ whenever the symmetric and antisymmetric localized eigenmodes were generated from the lower edge of the phonon band. We obtained explicitly the formula for the phonon transmission in the lowest order of the coupling strength. A perfect reflection was shown to exist...
at $k = \pi/2$ in the small coupling limit. The location of the perfect reflection was traced numerically until it disappeared through $k_c = 0$ at a critical value of the coupling strength.

The solution matching method using the transfer matrices has been proved to be an efficient tool for investigating scattering properties. Furthermore, the DNLS system provided a good intermediate example with two scattering channels bridging the gap between the case of a kink in the local equilibria with a single scattering channel and the discrete breather in the classical Hamiltonian system with an infinity of scattering channels. The methods used for the breather in the DNLS system can be extended to study the one-channel scattering of the nearest neighbor Hamiltonian chain. The multi-channel scattering problem is important in the context of stability, e.g., a two-channel scattering problem where the phonons of the second channel are incident from one side of the breather. Detail study of phonon-induced instability will be the subject of on-going investigations.

VI. ACKNOWLEDGMENTS

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FIG. 1. The eigenspectrum of linearized modes of the DNLS equation as a function of $\epsilon$. The phonon bands are shaded. The number in each region of the diagram denotes the number of the traveling channels.

(a) $0 < k_c < 1$

(b) $0 < -k_c < 1$

(c) same as (b)

FIG. 2. Continuation of the one-channel phonon-breather scattering configuration from a small positive value of $k_c$ to a small negative one.
FIG. 3. Phonon transmission through the breather in the DNLS equation in the weak-coupling limit. The solid line is the perturbative result, while diamonds denote the result of numerical calculations using the transfer matrix method.
FIG. 4. The blowup of Fig. VI with two branches of localized eigenmodes coming out of the phonon band.
FIG. 5. One-channel phonon transmissions through discrete breathers in the DNLS equation for $\omega = 1$. (a)-(b) Near $\epsilon = 0.262$ a perfect transmission is generated. (c)-(d) Near $\epsilon = 0.315$, the perfect transmission is annihilated.
FIG. 6. One-channel phonon transmissions through breathers in the DNLS equation for \( \omega = 1 \). Near \( \epsilon = 0.36 \), (a) the perfect reflection occurs at \( k \neq 0 \) or \( \pi \); (b) as the coupling strength is increased it is annihilated at \( k = 0 \). (c) The wave vector for the perfect reflection as a function of the coupling strength \( \epsilon \).