# Nonlinear spectral characterization of discrete data 

M. Boiti, ${ }^{1}$ J. Leon, ${ }^{2}$ and F. Pempinelli ${ }^{1}$<br>${ }^{1}$ Dipartimento di Fisica, Università di Lecce and Sezione INFN, I-73100 Lecce, Italy<br>${ }^{2}$ Physique Mathématique et Théorique, CNRS, F-34095 Montpellier, France

(Received 31 January 1996; revised manuscript received 23 May 1996)


#### Abstract

The explicit analytical expression of the nonlinear Fourier transform (NFT) of a finite set of data is provided. Then a simple recursion relation for the NFT is constructed as a function of the spectral parameter. These tools provide a complete characterization of the nonlinear coherent structures (solitons, breathers, ...) present in numerical or experimental data representing the solution, at a given value of time, of a nonlinear evolution equation (e.g., of the nonlinear Schrödinger family). [S1063-651X(96)12310-2]


PACS number(s): 03.40.Kf, 63.20.Pw

## INTRODUCTION

The inverse scattering (or spectral) transform (IST) is a method for constructing and solving nonlinear evolution equations (NEE) [1]. One of those, the nonlinear Schrödinger equation (NLS) [2], has become a paradigm as being the model for a wide variety of physical situations. Actually the relevant equation generally turns out to be nonintegrable, e.g., NLS with forcing and damping, which renders necessary a numerical analysis [3]. Then, a fundamental question is the characterization of the solution, as a standard Fourier analysis will not individualize the intrinsically nonlinear structures (as solitons). The same question is even more essential when dealing with experimental data.

Another fundamental aspect is the question of the discretization of an integrable continuous model, which raises many interesting questions such as numerical induced chaos [4], instabilities in integrable systems [5], or roundoff error growth [6].

Moreover, localized excitations (solitons) in nonlinear chains has been a subject of intense research for their obvious physical interest [7-9]. It has been proved, for instance, that the discreteness generically helps energy localization [10,11], that is, it is a mechanism controlling wave collapse [12], and also that it allows for the existence of moving localized modes [13] or standing ones [14].

In all these studies, the existence and properties of such localized excitations result merely from a direct observation of the numerical solution of the model. In short, a soliton is recognized from its shape, its velocity from the velocity of the point of maximum amplitude, the frequency of a breather is obtained from its Fourier spectrum, etc... .

However, there exists a tool, the nonlinear Fourier transform (NFT), which allows to characterize completely the nonlinear modes. It is based on IST and has been developed numerically either for the sine-Gordon family [15] to modelize fluxon dynamics in Josephson junctions, or for the Korteveg-de Vries model [16] to modelize water waves. In that case, the method has been successfully applied to experimental data [17], for instance, to prove that solitons $g e$ nerically occur in wave trains. The drawback, however, is on the one side the complexity of the method, and on the other side the lack of analytical formula for the NFT.

This paper is intended to provide two results, essential for
the nonlinear analysis of discrete data. The first one is an analytical explicit formula (11) for the NFT of a discrete set of data. More precisely, taking advantage of the finiteness of numerical or experimental data, we obtain the explicit expression of the Jost solutions, and hence of the complete spectrum characterization, corresponding to a discrete finite potential. The second one is a quite simple recursion relation (17) for a very straightforward numerical construction of the spectrum.

Everything is done in the context of the Ablowitz-Ladik spectral problem [18] (discrete version of the ZakharovShabat spectral problem), which means that the nonlinear Fourier analysis applies here for instance to the NLS family, that is,

$$
\begin{align*}
i \partial_{t} q(n)= & q(n+1)+q(n-1)-2 q(n) \\
& \pm|q(n)|^{2}[q(n+1)+q(n-1)]+a(n) \tag{1}
\end{align*}
$$

where $a(n)$ is any perturbation term. The method works without change for all nonintegrable deformations of the other integrable NEE related to the Ablowitz-Ladik spectral problem, such as mKdV , Toda, self-dual network, KdV, sine-Gordon [19], or discrete stimulated Raman scattering [20]. Lastly, the tool can be successfully applied to experimental data, as soon as the measurements are assumed to represent a train of envelope wave pulses which can be considered to vanish outside a finite interval. Indeed, in such a case the model equation for the envelope is likely to obey a member of the NLS family.

## STATEMENT OF THE PROBLEM

Given a finite discrete set of $2(L+1)$ complex valued data $q(n), r(n)$ having significant values on $n=0, \ldots, L$ and vanishing outside, the problem is to determine its nonlinear Fourier spectrum [the scalar case will enter as a reduction, e.g., $r=\mp \bar{q}$ to recover (1), where the overbar denotes complex conjugation]. This is done by using these data as the potential of the Ablowitz-Ladik scattering (or spectral) problem:

$$
\begin{gathered}
\mu_{11}(n+1)-\mu_{11}(n)=q(n+1) \mu_{21}(n+1), \\
\mu_{21}(n+1)-k^{-1} \mu_{21}(n)=r(n+1) \mu_{11}(n+1), \\
\mu_{12}(n+1)-k \mu_{12}(n)=q(n+1) \mu_{22}(n+1),
\end{gathered}
$$

$$
\begin{equation*}
\mu_{22}(n+1)-\mu_{22}(n)=r(n+1) \mu_{12}(n+1) \tag{2}
\end{equation*}
$$

for $n=-1, \ldots, L-1$. A dependence on the spectral parameter $k$ is understood everywhere for the matrix valued function $\mu(k, n)$ with elements $\mu_{i j}$.

The Jost solutions $\mu^{ \pm}$are then defined by the following discrete integral equations

$$
\begin{align*}
& \binom{\mu_{11}^{-}(n)}{\mu_{21}^{-}(n)}=\binom{1}{0}+\binom{-\sum_{i=n+1}^{L} q(i) \mu_{21}^{-}(i)}{\sum_{i=0}^{n} k^{i-n} r(i) \mu_{11}^{-}(i)},  \tag{3a}\\
& \binom{\mu_{11}^{+}(n)}{\mu_{21}^{+}(n)}=\binom{1}{0}-\binom{\sum_{i=n+1}^{L} q(i) \mu_{21}^{+}(i)}{\sum_{i=n+1}^{L} k^{i-n} r(i) \mu_{11}^{+}(i)},  \tag{3b}\\
& \binom{\mu_{12}^{-}(n)}{\mu_{22}^{-}(n)}=\binom{0}{1}-\binom{\sum_{i=n+1}^{L} k^{n-i} q(i) \mu_{22}^{-}(i)}{\sum_{i=n+1}^{L} r(i) \mu_{12}^{-}(i)},  \tag{3c}\\
& \binom{\mu_{12}^{+}(n)}{\mu_{22}^{+}(n)}=\binom{0}{1}+\binom{\sum_{i=0}^{n} k^{n-i} q(i) \mu_{22}^{+}(i)}{-\sum_{i=n+1}^{L} r(i) \mu_{12}^{+}(i)} . \tag{3d}
\end{align*}
$$

## NONLINEAR FOURIER SPECTRUM

The spectral transform of $\{q, r\}$ is then completely determined by the Jost solutions $\mu^{+}$and $\mu^{-}$as follows. An essential function is the reflection coefficient $\alpha^{ \pm}(k)$ defined as

$$
\begin{equation*}
\alpha^{-}=\sum_{0}^{L} k^{i} r(i) \mu_{11}^{-}(i), \quad \alpha^{+}=\sum_{0}^{L} k^{-i} q(i) \mu_{22}^{+}(i) . \tag{4}
\end{equation*}
$$

Due to the finiteness of the support of the potential $\{q, r\}$, the Jost eigenfunction, and hence $\alpha^{ \pm}(k)$, can be defined in the whole complex $k$ plane. Then the knowledge of the reflection coefficient in the complex plane allows one to determine completely the nonlinear Fourier spectrum, which consists of a continuous part (radiation) related to the values of $\alpha^{ \pm}$on the unit circle $|k|=1$, and of a discrete part (solitons) constituted by the poles $k_{j}^{-}$of $\alpha^{-}$in $|k|>1$ and $k_{j}^{+}$of $\alpha^{+}$in $|k|<1$. It is our purpose here to give an explicit formula for $\alpha^{ \pm}$in terms of the complex variable $k$.

## EXPLICIT SOLUTION

Introducing, for $(k, n)$, the new functions

$$
\begin{equation*}
\binom{\nu_{11}^{ \pm}}{\nu_{21}^{ \pm}}=\binom{\mu_{11}^{ \pm}}{k^{n} \mu_{21}^{ \pm}}, \quad\binom{\nu_{12}^{ \pm}}{\nu_{22}^{ \pm}}=\binom{k^{-n} \mu_{12}^{ \pm}}{\mu_{22}^{ \pm}}, \tag{5}
\end{equation*}
$$

the integral equations (3) become explicitly solvable in terms of the new matrix $\nu(k, n)$. This solution can be written in ( $k, n$ ),

$$
\begin{align*}
& \binom{\nu_{11}^{-}}{\nu_{21}^{-}}=X\binom{1}{\alpha^{-}}, \quad\binom{\nu_{11}^{+}}{\nu_{21}^{+}}=X\binom{1}{0},  \tag{6}\\
& \binom{\nu_{12}^{-}}{\nu_{22}^{-}}=X\binom{0}{1}, \quad\binom{\nu_{12}^{+}}{\nu_{22}^{+}}=X\binom{\alpha^{+}}{1} . \tag{7}
\end{align*}
$$

The matrix $X(n)$ reads

$$
X(n)=\prod_{i=n+1}^{L}\left(1-A_{i}\right), \quad A_{i}=\left(\begin{array}{cc}
0 & k^{-i} q(i)  \tag{8}\\
k^{i} r(i) & 0
\end{array}\right)
$$

with $X(L)=1$, or else

$$
X(n)=1-\sum_{\text {odd } l=1}^{L-n}\left(\begin{array}{cc}
0 & Q_{l}  \tag{9}\\
R_{l} & 0
\end{array}\right)+\sum_{\text {even } l=2}^{L-n}\left(\begin{array}{cc}
U_{l} & 0 \\
0 & V_{l}
\end{array}\right)
$$

with the following definitions of the functions of the two variables $(l, n)$ :

$$
\begin{align*}
& Q_{l}=\sum k^{-j_{1}} q\left(j_{1}\right) k^{j_{2}} r\left(j_{2}\right) \cdots k^{-j_{l}} q\left(j_{l}\right) \\
& R_{l}=\sum k^{j_{1}} r\left(j_{1}\right) k^{-j_{2}} q\left(j_{2}\right) \cdots k^{j_{l}} r\left(j_{l}\right) \\
& U_{l}=\sum k^{-j_{1}} q\left(j_{1}\right) k^{j_{2}} r\left(j_{2}\right) \cdots k^{j_{l}} r\left(j_{l}\right) \\
& V_{l}=\sum k^{j_{1}} r\left(j_{1}\right) k^{-j_{2}} q\left(j_{2}\right) \cdots k^{-j_{l}} q\left(j_{l}\right) \tag{10}
\end{align*}
$$

The sums run on all possible different $l$ indices $j_{i}$, ordered for each value of $(l, n)$ as $n+1 \leqslant j_{1}<j_{2}<\cdots<j_{l} \leqslant L$.

Then we may compute from $X(n)$ the reflection coefficients $\alpha^{ \pm}(k)$ which from their definition (4) read

$$
\begin{gather*}
\alpha^{-}(k)=\frac{\sum_{i=0}^{L} k^{i} r(i) X_{11}(i)}{1-\sum_{i=0}^{L} k^{i} r(i) X_{12}(i)}, \\
\alpha^{+}(k)=\frac{\sum_{i=0}^{L} k^{-i} q(i) X_{22}(i)}{1-\sum_{i=0}^{L} k^{-i} q(i) X_{21}(i)} . \tag{11}
\end{gather*}
$$

Note: the reduction $r(n)= \pm \bar{q}(n)$ leading, e.g., to the NEE (1), has the counterpart [20] $\alpha^{+}(1 / k)= \pm \alpha^{-}(\bar{k})$. These two relations are indeed compatible with (11).

## DATA RECONSTRUCTION

The data $\{r, q\}$ can be reconstructed from their spectral transform $\left\{\alpha^{+}, \alpha^{-}\right\}$because the solutions $\mu^{ \pm}(k, n)$ of (3) also solve [20]

$$
\begin{align*}
\binom{\mu_{11}^{ \pm}(k)}{\mu_{21}^{ \pm}(k)}= & \binom{1}{0}-\frac{1}{2 \pi i} \oint \frac{\zeta^{-n} d \zeta \alpha^{-}(\zeta)}{\zeta-(1 \mp 0) k} \frac{k}{\zeta}\binom{\mu_{12}^{-}(\zeta)}{\mu_{22}^{-}(\zeta)} \\
& +\sum_{j}\left(k_{j}^{-}\right)^{-n}{\operatorname{Res}\left\{\alpha^{-}\right\}}_{k_{j}^{-}}^{k_{j}^{-}} \frac{k}{k_{j}^{-}-k}\binom{\mu_{12}^{-}\left(k_{j}^{-}\right)}{\mu_{22}^{-}\left(k_{j}^{-}\right)}  \tag{12a}\\
\binom{\mu_{12}^{ \pm}(k)}{\mu_{22}^{ \pm}(k)}= & \binom{0}{1}+\frac{1}{2 \pi i} \oint \frac{\zeta^{n} d \zeta \alpha^{+}(\zeta)}{\zeta-(1 \mp 0) k}\binom{\mu_{11}^{+}(\zeta)}{\mu_{21}^{+}(\zeta)} \\
& -\sum_{j}\left(k_{j}^{+}\right)^{n} \operatorname{Res}\left\{\alpha^{+}\right\} \frac{1}{k_{j}^{+}-k}\binom{\mu_{11}^{+}\left(k_{j}^{+}\right)}{\mu_{21}^{+}\left(k_{j}^{+}\right)}, \tag{12b}
\end{align*}
$$

where the integral on $\zeta$ runs on the unit circle.
The system (2) at order zero in $k$ then gives

$$
\begin{equation*}
q(n+1)=-\mu_{12}^{-}(n)^{(-1)}, \quad r(n+1)=-\mu_{21}^{+}(n)^{(1)}, \tag{13}
\end{equation*}
$$

where $\mu_{12}^{-}(n)^{(-1)}$ is the coefficient of $k^{-1}$ in the Laurent expansion for $k \rightarrow \infty$ of $\mu_{12}^{-}(k, n)$, and $\mu_{21}^{+}(n)^{(1)}$ the coefficient of $k$ in the Taylor expansion for $k \rightarrow 0$ of $\mu_{21}^{+}(k, n)$.

These formulas are useful to prove the consistency of the method, that is, that the reconstructed data are the same as the starting ones (in particular, that they stay in the class of finite support). We do not develop this lengthy proof here but rather make the following remark: the above formulas allow one to filter the data just by setting to zero any part of the spectrum. For instance, if one needs information on the underlying nonlinear coherent structures, one may set to zero the contribution $\alpha^{ \pm}(\zeta),|\zeta|=1$ to the radiation, and then solve (12). Of course, doing this the reconstructed data do not stay in the class of finite support potentials, and this procedure will be meaningful for potentials going to zero fast enough at both ends.

## RECURSION RELATION

From its very definition (9), the matrix $X(n)$ can actually be considered as a function also of the variable $L$ (remember that $L$ is the dimension of the data support). We shall then denote it by $X^{L}(n)$ and, for instance, $X^{m}(n)$ has to be understood as obtained from the data of $\{q(n), r(n)\}$ for $n=0,1, \ldots, m$, and zero for $n \notin[0, m]$. Then our purpose here is to derive a recursion relation for the matrix elements of $X^{m}(n)$, in order to obtain a recursion relation for the corresponding spectral data $\alpha_{m}^{ \pm}(k)$, spectral transform of $\{q(n), r(n)\}$ for $n=0,1, \ldots, m$.

The spectral transform (11) is first conveniently rewritten as

$$
\begin{equation*}
\alpha_{m}^{-}=\frac{S_{m}}{1+\sum_{j=0}^{m-1} p_{j+1} S_{j}}, \quad \alpha_{m}^{+}=\frac{P_{m}}{1+\sum_{j=0}^{m-1} s_{j+1} P_{j}}, \tag{14}
\end{equation*}
$$

with the following definitions:

$$
\begin{gather*}
S(m)=\sum_{n=0}^{m} s(n) X_{11}^{m}(n), \quad P(m)=\sum_{i=0}^{m} p(n) X_{22}^{m}(n), \\
p(k, n)=k^{-n} q(n), \quad s(k, n)=k^{n} r(n) \tag{15}
\end{gather*}
$$

Then only the diagonal elements of $X^{m}(n)$ have to be considered.

By a careful rewriting of the element $X_{11}^{m+1}(n)$ out of (9), and by using that obviously $X_{11}^{n}(n)=X_{11}^{n+1}(n)=1$, we obtain

$$
\begin{equation*}
X_{11}^{m+1}(n)=X_{11}^{m}(n)+s(m+1) \sum_{j=n}^{m-1} p(j+1) X_{11}^{j}(n) \tag{16}
\end{equation*}
$$

A similar recursion relation is immediately deduced for $S(m)$ defined above, and consequently for $\alpha_{m}^{-}$. The same computation being made for $X_{22}^{m+1}(n)$ leads finally to

$$
\begin{array}{ll}
\alpha_{0}^{-}=r(0), & \alpha_{m+1}^{-}=\frac{s_{m+1}+\alpha_{m}^{-}}{1+p_{m+1} \alpha_{m}^{-}}, \\
\alpha_{0}^{+}=q(0), & \alpha_{m+1}^{+}=\frac{p_{m+1}+\alpha_{m}^{+}}{1+s_{m+1} \alpha_{m}^{+}} . \tag{17}
\end{array}
$$

If the data to be analyzed are given on [ $0, L$ ], the spectral transform $\alpha^{ \pm}(k)$ is constructed from the above recursion relation by running $m$ from 0 to $L$. To illustrate the preceding results we consider two examples.

## EXAMPLE 1: TWO-POINT DATA

In the case of two-point information ( $L=1$ ), by direct application of the above formula, we get

$$
\begin{equation*}
\alpha_{1}^{-}=\frac{r(0)+k r(1)}{1+k^{-1} q(1) r(0)}, \quad \alpha_{1}^{+}=\frac{q(0)+k^{-1} q(1)}{1+k q(0) r(1)} . \tag{18}
\end{equation*}
$$

An obvious and natural consequence is that two point data cannot represent a pure soliton solution which would require that $\alpha^{ \pm}$vanish on the unit circle $|k|=1$. The important information is that one can readily conclude about the presence of a soliton if $|q(1) r(0)|>1$ (which ensures a pole of $\alpha^{-}$in $|k|>1$ ) or/and if $|q(0) r(1)|>1$ (which ensures a pole of $\alpha^{+}$in $\left.|k|<1\right)$.

## EXAMPLE 2: TRUNCATED SOLITON

We consider the one soliton solution (reduction $r=-\bar{q}$ ) centered on $m=n_{0}$ and cut to the left of $m=0$ and to the right of $m=L$ defined by $\left(\eta_{0}, \theta_{0}\right.$ arbitrary constants and $b>0$ ),

$$
\begin{equation*}
q(m)=\frac{e^{i \eta_{0} m+\theta_{0}}}{\tau_{m}}, \quad \tau_{m}=\frac{\cosh \left(b m-b n_{0}\right)}{\sinh b} \tag{19}
\end{equation*}
$$

for $m=0,1, \ldots, L$ and $q(m)=0$ for $m<0$ and $m>L$. By using the recursion formula (17) the spectral transform can be explicitly computed giving ( $\xi=k e^{-i \eta_{0}}$ )

$$
\begin{equation*}
\alpha_{L}^{+}=-e^{i \theta_{0}} \xi^{-L} \frac{\xi^{L+2} \tau_{L}-\xi^{L+1} \tau_{L+1}-\left(\xi \tau_{-1}-\tau_{0}\right)}{\xi^{L+2}-\left(\xi \tau_{L+1}-\tau_{L}\right)\left(\xi \tau_{-1}-\tau_{0}\right)} \tag{20}
\end{equation*}
$$

A simple analysis for $L \gtrdot n_{0}$ shows that $\alpha_{L}$ has a pole for $|k|<1$ if and only if $n_{0}>0$. This means that the presence of a soliton in a wave train is detected with this method by analyzing only a finite portion of it. In the example considered, it is in fact enough to catch half of the soliton.

## CONCLUSION

The method is quite simple to use and it is of wide application: the formulas (11) provide an explicit function of the complex variable $k$ which allows one to completely characterize the nonlinear Fourier spectrum of the data
$\{r(n), q(n)\}$. In particular, the roots of the denominator of $\alpha^{-}$in the region $|k|>1$, and those of $\alpha^{+}$in $|k|<1$, furnish the nonlinear coherent structures present in the data. For practical applications, the recursion relations (17) provide a quite efficient numerical code to generate the nonlinear Fourier spectrum of any finite data. These relations possess a continuous counterpart, which will be studied, together with details and applications, in a forthcoming paper.

## ACKNOWLEDGMENTS

M.B. and F.P. are grateful to the Laboratoire de Physique Mathématique et Théorique for hospitality and to the CNRS for support. This work is part of the Contract Dynamique Nonlinéaire et Chaines Moléculaires - UM2.
[1] M.J. Ablowitz, D.J. Kaup, A.C. Newell, and H. Segur, Stud. Appl. Math. 53, 249 (1974); F. Calogero and A. Degasperis, Spectral Transform and Solitons (North Holland, Amsterdam, 1982); M. J. Ablowitz and P. Clarkson, Solitons, Nonlinear Evolutions and Inverse Scattering (Cambridge Univ. Press, Cambridge, 1992).
[2] V.E. Zakharov and A.B. Shabat, Zh. Éksp. Teor. Fiz. 61, 118 (1971) [Sov. Phys. JETP 34, 62 (1972)].
[3] V.G. Makhankov, Sov. J. Part. Nucl. 14, 50 (1983).
[4] B.M. Herbst and M.J. Ablowitz, Phys. Rev. Lett. 62, 2065 (1989).
[5] M.G. Forest, C.G. Goedde, and A. Sinha, Phys. Rev. Lett. 68, 2722 (1992).
[6] M.J. Ablowitz, C. Schober, and B.M. Herbst, Phys. Rev. Lett. 17, 2683 (1993).
[7] See e.g., M. Remoissenet, Waves Called Solitons (Springer, Berlin, 1995); Nonlinear Coherent Structures, edited by M. Barthes and J. Leon, Lecture Notes in Physics Vol. 353 (Springer, Berlin, 1990); Nonlinear Excitations in Biomolecules, edited by M. Peyrard (Les Editions de Physique, Springer, Berlin, 1995); Nonlinear Coherent Structures in Physics and Biology, edited by K.H. Spatschek and F.G. Mertens (Plenum, New York, 1994).
[8] M. Toda, Theory of Nonlinear Lattices (Springer, Berlin, 1981).
[9] A.J. Sievers and S. Takeno, Phys. Rev. Lett. 61, 970 (1988).
[10] T. Dauxois and M. Peyrard, Phys. Rev. Lett. 70, 3935 (1993); T. Dauxois, M. Peyrard, and C.R. Willis, Phys. Rev. E 48, 4768 (1993).
[11] S. Flach, K. Kladko, and C.R. Willis, Phys. Rev. E 50, 2293 (1994); S. Flach, ibid. 50, 3134 (1994).
[12] D. Cai, A.R. Bishop, and N. Gronbech-Jensen, Phys. Rev. Lett. 72, 591 (1994).
[13] Ch. Claude, Yu.S. Kivshar, O. Kluth, and K.H. Spatschek, Phys. Rev. B 47, 14228 (1993).
[14] Yu.S. Kivshar, M. Haelterman, and A.P. Sheppard, Phys. Rev. E 50, 3161 (1994).
[15] E.A. Overman II, D.W. McLaughlin, and A.R. Bishop, Physica D 19, 1 (1986); A.R. Bishop, M.G. Forest, D.W. McLaughlin, and E.A. Overman II, ibid. 23, 293 (1986).
[16] A.R. Osborne, J. Comp. Phys. 94, 284 (1991); A. Provenzale and A.R. Osborne, ibid. 94, 314 (1991); A.R. Osborne and E. Segre, Physica D 44, 575 (1990).
[17] A.R. Osborne, E. Segre, G. Boffetta, and L. Cavalieri, Phys. Rev. Lett. 67, 592 (1991).
[18] M.J. Ablowitz and J.F. Ladik, J. Math. Phys. 16, 598 (1975); 17, 1011 (1976).
[19] M.J. Ablowitz and H. Segur, Solitons and the Inverse Scattering Transform (SIAM, Philadelphia, 1981).
[20] M. Boiti, J. Leon, and F. Pempinelli, J. Math. Phys. 37, 2824 (1996).

