Rayleigh-Ritz procedure for the Zakharov-Shabat system

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The Rayleigh-Ritz variational procedure is applied to solve the Zakharov-Shabat scattering problem. An approximate solution is assumed as a linear combination of basis functions, leading to a homogeneous system of linear equations for eigenfunctions and an algebraic equation for eigenvalues. The effectiveness of the variational approach is illustrated by calculating the discrete spectrum of the Zakharov-Shabat system. Several numerical examples for various pulse-shaped potentials are given to demonstrate the practical usefulness of the method. [S1063-651X(97)12111-0]

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I. INTRODUCTION

The linear scattering problem

$$
v_{1,x} = -i\zeta v_1 + q(x)v_2, \qquad (1a)
$$

$$
v_{2,x} = r(x)v_1 + i\zeta v_2, \tag{1b}
$$

where $q(x)$, $r(x)$ are given potentials, v_1 , v_2 eigenfunctions, and ζ the corresponding eigenvalue, plays a major role in solving a variety of nonlinear evolution equations by means of the inverse scattering transform (IST) [1].

The system (1) with $r(x) = -q^*(x)$ was applied first by Zakharov and Shabat $\lceil 2 \rceil$ to solve the nonlinear Schrödinger (NLS) equation, and will be referred to as the ZS scattering problem. Subsequently, Ablowitz, *et al.* [1] used the system (1) to formulate the IST in a more general form, including such physically significant equations as Korteweg–de Vries, sine-Gordon, and others. The above equations can be applied to describe nonlinear phenomena in a wide variety of fields, including fluid dynamics, plasma physics, solid-state–lowtemperature physics, etc. In this paper, however, we shall focus our attention on the important applications in nonlinear optics, related to the propagation of soliton pulses in optical fibers.

In the context of nonlinear optics, the scattering potential plays a role of an initial pulse, and an important physical problem is to determine the soliton content of this pulse, i.e., to find the discrete spectrum of the system (1) . Unfortunately, apart from very few initial conditions, for which an exact solution exists, in a general case one has to use approximate methods $[3-7]$, such as direct numerical integration of Eqs. (1) or analytical approximations based, e.g., on the WKB method. Only recently, Desaix, Anderson, and Lisak $[8]$, and Kaup and Malomed $[9]$ have formulated independently a variational principle that can be used to solve the Zakharov-Shabat (ZS) system. In both papers mentioned above, the variational solution has been obtained using a simple ansatz for the eigenfunctions v_1 and v_2 .

The main advantage of such an approach is the possibility of obtaining an analytical approximate solution, dependent in a simple manner on a few variational parameters. However, the solution obtained this way agrees often only qualitatively with the exact solution and, in fact, we have no information concerning the error of approximation. Moreover, as a rule, a simple ansatz provides an estimate for a fundamental mode, while finding higher modes with reasonable accuracy requires much more complicated calculations.

On the other hand, there exist more systematic methods of the Rayleigh-Ritz (RR) type $[10]$, which are based on the series expansion of eigenfunctions and looking for a solution as a set of successive approximations. The main advantage of such a procedure is that the consecutive approximations tend to the exact solution, provided the basis set of the series expansion is complete. Thus, in spite of the fact that in practice we have to use finite expansions, it is possible to obtain rapid convergence and high numerical accuracy by a reasonable choice of basis functions.

Application of the RR procedure to the ZS system differs from the standard approach in quantum mechanics $[10]$. First, the ZS problem is non-self-adjoint, what implies that the eigenvalues are complex, and the stationary points of the appropriate functional are not its extremum values. Second, the ZS problem is a system of two equations for two eigenfunctions, i.e., a (2×2) matrix eigenproblem, leading to a $(2N\times2N)$ secular matrix. While the latter difficulty is of purely technical nature, the former one is essential and strongly influences the behavior of an approximate solution.

The aim of the present paper is twofold. First, we discuss application of the RR procedure to the ZS system in a more systematic way, clarifying some doubts related to the nonself-adjointness of the eigenproblem. Second, we present a few examples demonstrating the practical usefulness of the method, especially when the pulse area is at its threshold value for appearance of a new soliton.

The paper is organized as follows. In Sec. II the ZS equations are transformed to a non-self-adjoint eigenvalue problem. We find the adjoint operator, derive biorthogonality relations and show that the eigenvalues can be determined as stationary points of a functional equivalent to that reported in Refs. $\{8,9\}$. The RR procedure is described in Sec. III, both for a general case and for pulse shapes satisfying some symmetry relations. In Sec. IV we give numerical examples illustrating applicability of the RR procedure for various pulse shapes. In particular, the effect of chirping on the threshold amplitude (or area) is discussed in detail. Finally, Sec. V contains summary of the results and concluding remarks.

II. SPECTRAL PROBLEM AND VARIATIONAL FORMULATION

Let us consider the system (1) with a special choice $r(x) = -q^*(x)$, leading to the ZS scattering problem

$$
v_{1,x} = -i\zeta v_1 + q(x)v_2, \tag{2a}
$$

$$
v_{2,x} = -q^*(x)v_1 + i\zeta v_2, \tag{2b}
$$

where the eigenvalue $\zeta = \xi + i\eta$ is in general complex, and localized discrete eigenstates appear when η >0.

Rewriting Eqs. (2) in a matrix form we obtain the eigenproblem

$$
\mathcal{L}\Psi = \zeta \Psi,\tag{3}
$$

where

$$
\mathcal{L} = i \begin{bmatrix} \partial_x & -q \\ -q^* & -\partial_x \end{bmatrix}, \quad \Psi = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}.
$$

For the (real) scalar product

$$
(\Phi, \Psi) = \int_{-\infty}^{\infty} (\Phi^{\mathrm{T}} \cdot \Psi) dx, \tag{4}
$$

the adjoint problem is given by

$$
\widetilde{\mathcal{L}}\Phi = \mu\Phi,\tag{5}
$$

where

$$
\widetilde{\mathcal{L}} = i \begin{bmatrix} -\partial_x & -q^* \\ -q & \partial_x \end{bmatrix}, \quad \Phi = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}, \quad \mu = \zeta,
$$

and the eigenfunctions satisfy the biorthogonality condition

$$
(\Phi^{(i)}, \Psi^{(j)}) = 0, \qquad i \neq j. \tag{6}
$$

Let us consider the standard functional

$$
\mathcal{J}(\Phi, \Psi) = \frac{(\Phi, \mathcal{L}\Psi)}{(\Phi, \Psi)}.
$$
\n(7)

It is easy to check that $w_1 = v_2$, $w_2 = v_1$; thus coming back to v_1, v_2 functions we find

$$
\mathcal{J}(v_1, v_2) = i \frac{\int_{-\infty}^{\infty} [(v_{1,x}v_2 - v_{2,x}v_1) - (qv_2^2 + q^*v_1^2)]dx}{2 \int_{-\infty}^{\infty} v_1v_2 dx},
$$
\n(8)

which is equivalent to the functionals given in Refs. $[8,9]$.

It can be easily verified that the variation δJ vanishes for v_1, v_2 satisfying Eqs. (2), and the value of the functional corresponds to the eigenvalue ζ . However, contrary to selfadjoint problems now at the stationary point neither real nor imaginary part of ζ attains an extremum.

For given initial pulse shape $q(x)$, the eigenproblem has a finite number of discrete states and the continuous spectrum. The fundamental mode (designated by $i=0$) appears at the lowest pulse area at the threshold value $\eta=0$. For higher pulse areas additional (higher) modes emerge at $\eta=0$, and $n^{(0)} > n^{(1)} > n^{(2)} > \cdots$. Thus, the stationary point $\delta J = 0$, for which we obtain the largest eigenvalue corresponds to the fundamental mode. Subsequent (higher) modes can be found for the stationary points subject to additional orthogonality conditions:

$$
(\Phi^{(j)}, \Psi) = 0, \qquad j = 0, 1, 2, \dots, (i - 1), \tag{9}
$$

where *i* denotes the mode number for a higher eigenvalue or eigenfunction to be determined. We note also that the fundamental eigenfunctions have $i=0$ nodes, while higher modes correspond to *i* nodes for each eigenfunction v_1, v_2 .

III. RR PROCEDURE AND THE SYMMETRY RELATIONS

From the numerical viewpoint it is convenient to transform the functional (8) to an equivalent form

$$
\widetilde{\mathcal{J}}(v_1, v_2) = \int_{-\infty}^{\infty} [(v_{1,x}v_2 - v_{2,x}v_1) - (qv_2^2 + q^*v_1^2)]dx
$$

+2i\zeta \int_{-\infty}^{\infty} v_1v_2dx, (10)

and consider trial functions in a form of series expansions,

$$
v_1 = \sum_n a_n \phi_n, \quad v_2 = \sum_n b_n \psi_n, \tag{11}
$$

where ϕ_n , ψ_n are two (generally different) complete sets of basis functions, and a_n , b_n are expansion coefficients to be determined.

Substituting expansions (11) to the functional (10) , and making the derivatives $\partial J/\partial a_n$, $\partial J/\partial b_n$ equal to zero, we obtain a system of homogenous linear equations with respect to a_n and b_n . If we replace infinite expansions (11) by finite sums consisting of *N* terms, the resulting secular $(2N\times2N)$ matrix will have the following block form:

$$
\left[\begin{array}{cc} A & B \\ C & D \end{array}\right],\tag{12}
$$

where the matrix elements are given by

$$
A_{nm} = \int_{-\infty}^{\infty} (\phi_{m,x} \psi_n - \phi_m \psi_{n,x}) dx + 2i \zeta \int_{-\infty}^{\infty} \phi_m \psi_n dx,
$$
\n(13a)

$$
B_{nm'} = -2 \int_{-\infty}^{\infty} q \psi_n \psi_{m'} dx, \quad m' = m - N, \qquad (13b)
$$

$$
C_{n'm} = -2 \int_{-\infty}^{\infty} q^* \phi_{n'} \phi_m dx, \quad n' = n - N, \quad (13c)
$$

$$
D_{n'm'} = \int_{-\infty}^{\infty} (\phi_{n',x}\psi_{m'} - \phi_{n'}\psi_{m',x})dx + 2i\zeta \int_{-\infty}^{\infty} \phi_{n'}\psi_{m'}dx.
$$
\n(13d)

Making the determinant of Eq. (12) equal to zero, we obtain an algebraic equation for the eigenvalue to be determined. Next, by increasing *N* we can form a sequence of consecutive approximations tending to the exact solution if $N \rightarrow \infty$.

As mentioned in the preceding section, for given initial pulse $q(x)$ the fundamental mode corresponds to the largest stationary value η . Next solutions can be found by looking for a stationary point of the functional (7) at the additional orthogonality conditions (9) introduced to the functional, e.g., by the Lagrange multiplier method. However, if we fix *N*, calculate approximately $\zeta^{(0)}, \upsilon_1^{(0)}, \upsilon_2^{(0)}$, and take $\Phi^{(0)}$ as a fundamental mode in Eq. (9) , it can be shown [11] that the next solution $\zeta^{(1)}$ will be identical with the next zero of the secular determinant of Eq. (12). Thus, instead of introducing additional orthogonality conditions, we can find higher modes simply by looking for consecutive zeros of the secular determinant.

So far, we have considered a general form of an initial pulse $q(x)$ and independent expansions (11). For $q(x)$ satisfying certain symmetry conditions it is possible to find simple relations between v_1 and v_2 . Below, we discuss briefly only two such symmetries.

(i) Substituting

$$
q(-x) = q(x) \tag{14}
$$

into Eqs. (2) we find

$$
v_2(x) = pv_1^*(-x), \qquad p = \pm 1. \tag{15}
$$

It can be deduced from symmetry considerations that $p=-1$ for the fundamental mode, $p=+1$ for the first higher mode, etc. Assuming $\psi_n(x) = p \phi_n(-x)$ we find expansion coefficients to satisfy the relation $b_n = a_n^*$, while the eigenvalue ζ is purely imaginary or appears in complex-conjugate pairs.

~ii! For

$$
q(-x) = q^*(x) \tag{16}
$$

we have simply

$$
v_2(x) = pv_1(-x), \qquad p = \pm 1, \tag{17}
$$

where $p=-1$ for the fundamental mode, as before.

For $\psi_n(x) = p \phi_n(-x)$ expansion coefficients are related by $b_n = a_n$; hence, the matrix expressions can be substantially simplified. Indeed, for *N* fixed we obtain a $(N \times N)$ secular matrix, with elements given by

$$
A_{nm} = \int_{-\infty}^{\infty} [(\phi_{n,x}\psi_m - \phi_n\psi_{m,x}) - (q\psi_n\psi_m + q^*\phi_n\phi_m)]dx
$$

+ $i\zeta \int_{-\infty}^{\infty} (\phi_n\psi_m + \psi_n\phi_m)dx.$ (18)

IV. NUMERICAL EXAMPLES

A. Boxlike pulse

Let us consider first an example $[9]$ for which exact analytic solution exists,

TABLE I. Complex eigenvalues $\zeta = \xi + i\eta$ for the boxlike potential (19), $A=1$, $\epsilon=1$. Successive approximations for *N* up to 50 are shown together with the exact solution.

Ν	ξ	η
10	-0.76119	0.124 79
20	-0.76150	0.124 39
30	-0.76144	0.124 44
40	-0.76146	0.12442
50	-0.76145	0.124 43
exact	-0.761453	0.124 429

$$
q = \begin{cases} A \exp(i\epsilon) & \text{for } 0 < x < a \\ A \exp(-i\epsilon) & \text{for } -a < x < 0 \\ 0 & \text{for } |x| > a. \end{cases}
$$
 (19)

Asymptotics of the Jost functions for a localized solution of Eqs. (2) implies that

$$
v_1 \rightarrow \exp(-i \zeta x), v_2 \rightarrow 0, \text{ as } x \rightarrow -\infty,
$$
 (20a)

$$
v_1 \rightarrow 0
$$
, $v_2 \rightarrow \exp(i\zeta x)$, as $x \rightarrow \infty$. (20b)

In particular, for a potential $q(x)$ on a compact support we have exactly $v_2=0$ for $x<-a$ and $v_1=0$ for $x>a$. Thus, it is natural to choose the basis set

$$
\phi_n = \sin\left[(2n-1)\frac{\pi}{4} \left(1 - \frac{x}{a} \right) \right],\tag{21a}
$$

$$
\psi_n = p \sin \left[(2n-1) \frac{\pi}{4} \left(1 + \frac{x}{a} \right) \right], \quad p = \pm 1. \tag{21b}
$$

The potential (19) satisfies the symmetry relation (16) ; thus, we can use a reduced form of the secular matrix (18) . Numerical results for finite expansions including up to $N=50$ terms are presented in Tables I and II, to show the convergence of the method. The exact analytical solution follows from matching trigonometric functions at $x=0,\pm 1$ and next solving the resulting transcendental equation for $\zeta = \xi + i \eta$. A physically meaningful solution must vanish at infinity; hence, the asymptotic behavior (20) requires η >0 for a localized state.

TABLE II. Complex eigenvalues $\zeta = \xi + i\eta$ for the boxlike potential (19), $A=2$, $\epsilon=1$. Successive approximations and exact solutions are shown for the fundamental $(i=0)$ and the first higher mode $(i=1)$.

	$i=0$		$i=1$	
N	ξ	η	ξ	η
10	-0.72789	1.210.65	0.981 00	0.396 99
20	-0.72848	1.210 35	0.981 29	0.396 74
30	-0.72823	1.210 35	0.980 98	0.39685
40	-0.72827	1.210 34	0.981 02	0.39683
50	-0.72824	1.210.34	0.980 98	0.39684
exact	-0.728241	1.210 342	0.980 980	0.396 842

TABLE III. Threshold values A_{thr} and the shifts ΔA for the boxlike potential (22) and the chirp parameter β changing from 0 to 0.1. Results for the first three modes are shown.

		$A_{\rm thr}$	
Mode	$\beta = 0$	β =0.1	ΔΑ
0	0.78540	0.78586	0.00046
	2.356 19	2.355 90	-0.00029
$\mathfrak{D}_{\mathfrak{p}}$	3.926.99	3.926.61	-0.00038

For $A=1$, $\epsilon=1$ (Table I) only one localized state exists, while for $A=2$, $\epsilon=1$ (Table II) we obtain two solutions satisfying η > 0 and calculated with comparable accuracy.

A more realistic model is a boxlike pulse with a chirp $[3]$,

$$
q = \begin{cases} A \exp(i\beta x^2) & \text{for} \quad |x| < a, \\ 0 & \text{for} \quad |x| > a. \end{cases} \tag{22}
$$

This time, due to symmetry relation (14) the resulting eigenvalues are purely imaginary; however, we have to use the full $(2N\times2N)$ matrix (12) .

It is interesting to investigate threshold values of the pulse amplitude A_{thr} (or equivalently, pulse area), such that a new soliton emerges at $\eta=0$. It should be noted that in the vicinity of the threshold the eigenfunctions v_1, v_2 are weakly localized, and for $\eta \rightarrow 0$ their amplitudes tend to constant values as $|x| \rightarrow \infty$ [see Eq. (20)]. Such a behavior may cause numerical instabilities for $n \approx 0$, especially when solving Eqs. (2) by direct numerical integration.

Fortunately, in the variational approach this difficulty does not appear, since the regions outside of $|x|=a$ do not contribute to the integrals in Eq. (10) . As a result, we obtain stable numerical solutions in the vicinity of the threshold. Moreover, it is formally possible to obtain even nonphysical solutions with η <0, i.e., for eigenfunctions divergent as $|x|$ →∞.

In Table III the threshold values A_{thr} are shown for the first three modes, together with the shift $\Delta A = A_{\text{thr}}|_{\beta=0.1} - A_{\text{thr}}|_{\beta=0}$. It is clear that the effect of chirp for small β is rather subtle, so accurate calculations are required. We note, that $\Delta A > 0$ for the fundamental mode, while $\Delta A \leq 0$ for higher modes, in agreement with earlier results $\lfloor 3 \rfloor$.

B. Sech pulse

Let us consider a sech pulse with a chirp

$$
q = A \, \text{sech}(x) \exp(i\beta x^2). \tag{23}
$$

As before, a physically interesting problem is the soliton content of the pulse, as well as the influence of a chirp on threshold values of amplitude (or pulse area).

Now however, *q* is not on a compact support, and a numerical problem arises, how to reconstruct eigenfunctions v_1, v_2 in the infinite region ($-\infty, \infty$). This problem becomes more pronounced in the vicinity of $\eta=0$, when the eigenfunctions cease to be localized.

We have checked various methods of approximation on the infinite interval, such as $e.g.$ (i) using Hermite polynomi-

TABLE IV. Imaginary part η of the eigenvalue for the sech pulse (23), $A=1$ and $\beta=0$, $\beta=0.8$.

		η	
N	$\beta = 0$	β =0.8	
10	0.475 58		
20	0.499 63	0.012 03	
30	0.500 00	0.01936	
40	0.500 00	0.019 57	
50	0.500 00	0.01960	

als which form a basis set complete for $(-\infty,\infty)$ or (ii) projecting the *x* axis onto the finite interval.

In all the cases one could obtain accurate results for welllocalized solutions (far above the threshold). However, as the eigenvalue was close to zero, the convergence deteriorated rapidly, and we were not able to obtain reliable results for $n\approx0$.

It turns out, however, that the best and simultaneously the simplest method is an apparently crude approximation consisting in "truncating" the potential q for sufficiently large |x| values and using the basis set of the type (21) on a finite interval. The choice of the cut-off point $|x| = a$ depends on the pulse shape and is a compromise between required accuracy and sufficiently fast convergence. For example, for the sech pulse we have chosen $a=10$ to obtain reasonable convergence and the absolute error estimated below 10^{-5} .

In Table IV we show examples of calculations for a sech pulse (23) with A=1, and $\beta=0$, $\beta=0.8$, respectively. According to general symmetry considerations, the eigenvalue ζ is now purely imaginary. For $\beta=0$ we obtain the exact solution $\eta=0.5$. As β increases the eigenvalue η decreases and the convergence becomes slower. Nevertheless, also for $\eta \approx 0$ we obtain stable results. In particular, for $A=0.75$, 0.5, 1.25 we find the threshold $\eta=0$ at β =0.4203, 0.8220, 1.2391, respectively, in excellent agreement with the literature data $[5]$.

To compare the sech pulse with the boxlike case, we have calculated the threshold amplitudes A_{thr} and the shifts ΔA for β changing from 0 to 0.1. The results for ΔA are presented in Table V together with similar calculations performed for other pulse shapes. We can see that the absolute shift ΔA is

TABLE V. Shifts ΔA of the threshold amplitude A_{thr} for the chirp parameter β changing from 0 to 0.1. Comparison is made for the first three modes and various pulse shapes.

		ΔΑ		
Mode	Box ^a	Sech ^b	Sech ^c	Gaussian ^d
θ	0.00046	0.0419	0.0107	0.00264
	-0.00029	0.0652	0.0006	0.001 68
	-0.00038	0.0752	-0.0037	0.00134

 ${}^{\text{a}}$ Equation (22).

 b Equation (23).</sup>

 c Equation (24) .

 d Equation (25).

much larger for the sech pulse, and contrary to the box-like case all the shifts are positive.

It is clear from Eq. (23) that for large x the chirp factor $exp(i\beta x^2)$ is rapidly oscillating, what may be a source of numerical instabilities. In order to avoid such difficulties an alternative form has been suggested in Ref. $[3]$:

$$
q = A \ \operatorname{sech}(x) \exp\left(\frac{i\beta x^2}{1 + \alpha x^2}\right). \tag{24}
$$

Contrary to the previous model (23) , now the phase tends to a constant and the chirp vanishes as $|x| \rightarrow \infty$. The constant α depends on the pulse shape and for the sech pulse has been arbitrarily chosen as $\alpha = 1/12$ [3].

The shifts ΔA calculated for the pulse shape (24) are shown in the fourth column of Table V. These values of ΔA (after appropriate scaling to make the notation consistent) are in a very good agreement with the results obtained by the perturbation method $[3]$. As compared to the pulse shape (23) , when all the shifts were positive, now we observe substantially smaller values, and moreover, ΔA changes its sign for the second mode. Thus, one can conclude that the anomalous behavior of the shifts ΔA reported in Ref. [3] is not a characteristic property of the sech pulse, but follows rather from the assumed form of the chirp factor.

C. Gaussian pulse

Numerical procedures for the Gaussian pulse are essentially the same as for the sech pulse, with the form (23) replaced by

$$
q = A \exp(-\sigma^2 x^2) \exp(i\beta x^2). \tag{25}
$$

Due to faster decay as $|x| \rightarrow \infty$ we can "cut off" the potential *q* at smaller values of *a*, obtaining this way a better convergence.

The last column of Table V shows the shifts ΔA calculated for the Gaussian pulse with $\sigma=1$ and $a=4$. We can see that all the shifts are again positive, however, the absolute values are lower than in the sech case, what means that for the Gaussian shape the chirp affects less the soliton content of the initial pulse.

V. CONCLUDING REMARKS

In the present paper we have discussed possible application of the Rayleigh-Ritz procedure for solving the non-selfadjoint eigenvalue problem (2) . The effectiveness of the method has been illustrated by giving numerical examples for several initial pulses with a chirp. In particular, it has been shown that the method is numerically stable and yields reliable results also in the vicinity of the threshold $\eta=0$ when the eigenfunctions cease to be localized and many other approximate methods fail. Investigating the influence of the chirp on the threshold amplitude *A*thr we have shown that for a boxlike pulse, chirping causes A_{thr} to increase for the fundamental mode $(\Delta A > 0)$, while $\Delta A < 0$ for higher modes. Contrary to the box case, for pulses with long tails (sech and Gaussian) we observe $\Delta A > 0$ for both fundamental and higher modes. It should be stressed, however, that the threshold amplitudes are very sensitive to the assumed form of the chirping factor. For example, assuming the shape (24) instead of (23) not only makes the shifts ΔA much smaller, but also reverses the sign of ΔA for the second mode.

Summarizing, one can conclude that the Rayleigh-Ritz procedure yields accurate and numerically stable results for various pulse shapes (potentials) $q(x)$. In particular, it is possible to determine the soliton content of the initial pulse and predict precisely the threshold amplitude for appearance of a new soliton. Thus, the discussed Rayleigh-Ritz procedure may be an interesting alternative to other approximate methods of solving the ZS problem, both based on variational approach and using direct numerical integration of the system (2) .

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