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Numerically Induced Phase Shift in the KdV Soliton

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When using a finite difference scheme to study the motion of a KdV soliton, a shift in the position of the soliton from the exact solution is detected. In this paper we retain the lowest order terms in the truncation error and treat them analytically as a perturbation of the KdV equation. It is found that perturbation theory can be used to determine the numerically induced shift. © 1993 Academic Press, Inc.

INTRODUCTION

The Korteweg-de Vries (KdV) equation, given by

$$u_t + 6uu_x + u_{xxx} = 0, \tag{1}$$

appears in many physical contexts; for example, it can be derived from the study of water waves [7, 8], or ion-acoustic waves in plasma [13]. Special solutions to the equation have been known for over 100 years, but it was only 25 years ago that a method was developed for solving the initial value problem. This method, now known as the inverse scattering transform (IST), was introduced by Gardner *et al.*, 1967 [2]. Their discoveries were motivated by a numerical study of the KdV equation conducted by Zabusky and Kruskal in 1965 [14]. Zabusky and Kruskal found that an initial profile evolved into a train of solitary waves each of which behaved like a particle. During collisions the solitary waves interacted nonlinearly and then they emerged with their identities preserved. Zabusky and Kruskal called these solitary waves *solitons*. A simple analytical form for the KdV soliton is given by

$$u(x, t) = 2\eta^2 \operatorname{sech}^2 \eta(x - 4\eta^2 t), \tag{2}$$

where η is a positive real constant. It is easily seen that this solution has amplitude $2\eta^2$, width $1/\eta$, and center $x_c = 4\eta^2 t$. In comparing the numerical results from the Zabusky-Kruskal scheme with (2) we find that all of the features of the soliton are accurate with the exception of the soliton center. As shown in Fig. 1, at time $t = 20$, the computer generated soliton lags behind the analytic soliton by 5%. The question is then: Why is the numerical soliton moving slower than expected? This phase shift has been noted by several authors including Sanz-Serna [11] and Knickerbocker [7].

In this paper we will use perturbation theory to analytically study the effects of the truncation error for the Zabusky-Kruskal scheme on a single soliton and we will show that this discretization error does account for the numerically induced phase shift. In the next section we present the finite difference scheme and compute the truncation error. In the sections to follow we use singular perturbation theory to predict the changes to the soliton including the location of the soliton, and in the last section we make a comparison of the numerical and theoretical results. A byproduct of this study is a simple modification of the Zabusky-Kruskal scheme, which can be implemented in the same amount of time with more accurate results.

TRUNCATION ERROR FOR THE ZABUSKY-KRUSKAL SCHEME

In 1965 Zabusky and Kruskal [14] studied the KdV equation numerically using a periodic initial condition. The finite difference scheme they used, hereafter referred to as the ZK scheme, can be summarized by the equations

$$u_t = \frac{u(j, n+1) - u(j, n-1)}{2\Delta t} + O(\Delta t^2) \tag{3}$$

$$u = \frac{u(j+1, n) + u(j, n) + u(j-1, n)}{3} + O(\Delta x^2) \tag{4}$$

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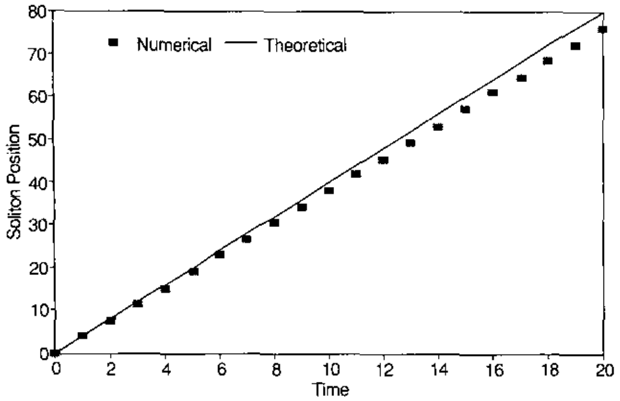

FIG. 1. Comparison of the numerical and theoretical positions of the soliton peak for $\eta = 1$, $\Delta x = 0.5$, $\Delta t = 0.03125$.

$$u_x = \frac{u(j+1, n) - u(j-1, n)}{2\Delta x} + O(\Delta x^2) \tag{5}$$

$$u_{xxx} = \frac{\begin{pmatrix} u(j+2, n) - 2u(j+1, n) \\ \quad + 2u(j-1, n) - u(j-2, n) \end{pmatrix}}{2\Delta x^3} + O(\Delta x^2), \tag{6}$$

where $t = n\,\Delta t$ and $x = j\,\Delta x$. Vliegenthart [12] studied this scheme and found that the linear stability condition is given by

$$\Delta t \leqslant [6\Delta x\,|u| + 4(\Delta x)^{-3}]^{-1}. \tag{7}$$

However, implementation of the scheme can be accomplished by requiring

$$\Delta t = (\Delta x)^3/4. \tag{8}$$

The leading order terms for the truncation error can be obtained by using Taylor expansions. Denoting the numerical solution by $\tilde{u}$, and the actual solution by u, we can rewrite the numerical scheme as

$$\tilde{u}_t = \frac{u(t+\Delta t) - u(t-\Delta t)}{2\Delta t} \approx u_t + \frac{1}{6}\Delta t^2\, u_{ttt} \tag{9}$$

$$\tilde{u} = \frac{u(x+\Delta x) + u(x) + u(x-\Delta x)}{3}$$

$$\approx u + \frac{1}{3}\Delta x^2\, u_{xx} \tag{10}$$

$$\tilde{u}_x = \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x}$$

$$\approx u_x + \frac{1}{6}\Delta x^2\, u_{xxx} \tag{11}$$

$$\tilde{u}_{xxx} = \frac{\begin{pmatrix} u(x+2\Delta x) - 2u(x+\Delta x) \\ \quad + 2u(x-\Delta x) - u(x-2\Delta x) \end{pmatrix}}{2\Delta x^3}$$

$$\approx u_{xxx} + \frac{1}{4}\Delta x^2\, u_{xxxxx}. \tag{12}$$

Thus, numerically one is solving

$$0 = \tilde{u}_t + 6\tilde{u}\tilde{u}_x + \tilde{u}_{xxx}$$

$$\simeq u_t + 6uu_x + u_{xxx} + E(u), \tag{13}$$

where the truncation error for the equation is defined as

$$E(u) = \tfrac{1}{6}\Delta t^2\, u_{ttt} + \Delta x^2\,\{2u_x u_{xx} + uu_{xxx} + \tfrac{1}{4}u_{xxxxx}\}. \tag{14}$$

Therefore, by using the ZK scheme, we are actually solving to leading order a perturbed KdV equation

$$u_t + 6uu_x + u_{xxx} = -\tfrac{1}{6}\Delta t^2\, u_{ttt} - \Delta x^2\{2u_x u_{xx} + uu_{xxx} + \tfrac{1}{4}u_{xxxxx}\}. \tag{15}$$

If we define a small parameter $\varepsilon = \Delta x^2$, then we find from the stability condition (8) that $\Delta t^2 \simeq \varepsilon^3/4$. Therefore, the first term in the perturbation is of much higher order in ε than the other terms. So, we can study the perturbed KdV equation

$$u_t + 6uu_x + u_{xxx} = -\varepsilon\{2u_x u_{xx} + uu_{xxx} + \tfrac{1}{4}u_{xxxxx}\}, \tag{16}$$

in order to determine if the discrepancy in the soliton position in Fig. 1 can be predicted.

ANALYSIS OF PERTURBED KDV EQUATIONS

In the last section we obtained a perturbed KdV equation, which contains the leading order corrections due to the truncation error present in the ZK scheme. We now turn to the perturbation theory developed for the KdV equation and see if we can account for the observed shift in the soliton position.

Since the mid 1970s several papers were produced to describe the effects of perturbations on soliton solutions of integrable nonlinear evolution equations [3–6, 9]. Kaup [5] had suggested the use of IST to study singular perturbations of these equations. Later Kaup and Newell (KN [6] had applied this method to the KdV equation, as well as other perturbed equations. At the same time Karpman and Maslov (KM) had also used similar methods to study perturbations of the KdV equation [4]. It was found from these studies that the effects of small perturbations could lead to a change in the shape and position, or phase shift, of the initial soliton, as well as the formation of a secondary structure behind the soliton.

There are some discrepancies between these two approaches [3]. Also, further analysis of such numerical schemes, using perturbation theory, should involve an accurate determination of the first-order correction to the solution. For these reasons, we will present a more natural approach towards viewing the perturbation problem at hand. We will consider a direct approach for solving the perturbed equation [3]

$$u_t + 6uu_x + u_{xxx} = \varepsilon F[u], \tag{17}$$

subject to the initial condition

$$u(x, 0) = 2\eta^2 \operatorname{sech}^2 \eta x. \tag{18}$$

This method differs from the above IST methods in that we will study the effects of the perturbations in physical space and not in spectral space. From these results we will be able to predict the effects of the truncation error on the propagation of the soliton. We will find that the perturbation term in (17) can potentially affect the shape and location of the soliton. As we are not interested in the stability of the scheme, we will only provide the form for the first-order correction, reserving such a discussion for a later paper in which several numerical schemes are nalyzed.

For small perturbations, we expect that the solution will remain close to the soliton solution for some time. Therefore, the solution we seek will be a solitary wave with a slowly changing shape and location plus a correction. In order to accomplish this, we will assume an asymptotic expansion of the form

$$u(x, t) = u_0(x, t) + \varepsilon u_1(x, t) + \cdots, \tag{19}$$

where we take

$$u_0(x, t) = 2\eta^2 \operatorname{sech}^2 \eta \left(x - \frac{1}{\varepsilon} x_0 - x_1 \right). \tag{20}$$

We will also assume that the soliton parameters are slowly varying. In order to accomplish this we define the two time scales, $T = t$ and $\tau = \varepsilon t$, and we allow η, x_0, and x_1 to depend only on the slow scale τ.

Introducing the expansion (19) and the two time scales into Eq. (17), we obtain an expansion of (17) in powers of ε. Setting the coefficients of each order of ε to zero, we obtain a system of equations to be solved for u_n. The lowest order equation is the KdV equation, which will be satisfied if

$$x_{0_\tau} = 4\eta^2. \tag{21}$$

The first-order equation then becomes

$$\mathscr{L}u_1 = -4\eta\eta_\tau v - 2\eta\eta_\tau \phi v_\phi + 2\eta^3 x_{1_\tau} v_\phi + F[u_0], \tag{22}$$

where $\mathscr{L}$ is the linearized KdV operator

$$\mathscr{L} \equiv \partial_T - 4\eta^3 \partial_\phi + 6\eta \partial_\phi u_0 + \eta^3 \partial_\phi^3, \tag{23}$$

and

$$v \equiv \operatorname{sech}^2 \phi$$
$$\phi \equiv \eta(x - x_0/\varepsilon - x_1).$$

The problem is now to invert this operator. The details of this inversion for the general problem

$$\mathscr{L}u_1 = \mathscr{F} \tag{24}$$

is presented in [3]. Summarizing this method, we expand the correction u_1 in a complete set of basis states, $\{\Phi^A, \Phi_1^A, \Lambda_1^A\}$,

$$u_1 = \int_{-\infty}^{\infty} d\lambda\, f(\lambda, t)\, \Phi^A(x, t; \lambda) + f_1(t)\, \Phi_1^A(x, t) + g_1(t)\, \Lambda_1^A(x, t). \tag{25}$$

In Appendix A we list the forms for this basis and its corresponding adjoints, $\{\Phi, \Phi_1, \Lambda_1\}$, for the one soliton case. Employing the orthogonality relations between these sets [3], we obtain the expansion coefficients

$$f(\lambda, t) = \int_0^t dt' \frac{\langle \mathscr{F} \mid \Phi \rangle}{2\pi i \lambda a^2(\lambda)} e^{8i\lambda^3(t-t')} \tag{26}$$

$$g_1(t) = -2i\eta \int_0^t dt' \langle \mathscr{F} \mid \Phi_1 \rangle e^{8\eta^3(t-t')} \tag{27}$$

$$f_1(t) = -2i\eta \int_0^t dt' \langle \mathscr{F} \mid \Lambda_1 \rangle e^{8\eta^3(t-t')} - 96\eta^3 \int_0^t dt' \int_0^{t'} dt'' \langle \mathscr{F} \mid \Phi_1 \rangle e^{8\eta^3(t-t'')}, \tag{28}$$

where the inner product is defined by

$$\langle f(x) \mid g(x) \rangle \equiv \int_{-\infty}^{\infty} f(x)\, g(x)\, dx. \tag{29}$$

Using the basis states for a one-soliton solution, we can rewrite the last two terms in (25),

$$B \equiv f_1 \Phi_1^A + g_1 \Lambda_1^A, \tag{30}$$

as

$$B = \tilde{g}_1[\operatorname{sech}^2\phi + \tfrac{1}{2}\phi(\operatorname{sech}^2\phi)_\phi] + \tilde{h}_1(\operatorname{sech}^2\phi)_\phi, \tag{31}$$

where the new coefficients are given by

$$\tilde{g}_1 \equiv \int_0^t dt' \, \langle \mathscr{F} \,|\, \operatorname{sech}^2\phi \rangle \tag{32}$$

$$\tilde{h}_1 \equiv -\tfrac{1}{2}\int_0^t dt' \, \langle \mathscr{F} \,|\, [\phi + 8\eta^3(t-t')] \times \operatorname{sech}^2\phi + \tanh\phi \rangle. \tag{33}$$

We note that for $\mathscr{F}$ independent of time these coefficients will grow in time, unless we impose the secularity conditions

$$\langle \mathscr{F} \,|\, \operatorname{sech}^2\phi \rangle = 0 \tag{34}$$

$$\langle \mathscr{F} \,|\, \phi \operatorname{sech}^2\phi + \tanh\phi \rangle = 0. \tag{35}$$

Applying these conditions to Eq. (22), we obtain the slow time dependence of the soliton parameters [3]:

$$\eta_\tau = \frac{1}{4\eta}\int_{-\infty}^{\infty} F[u_0] \operatorname{sech}^2\phi \, d\phi \tag{36}$$

$$x_{0\tau} = -4\eta^2 \tag{37}$$

$$x_{1\tau} = \frac{1}{4\eta^3}\int_{-\infty}^{\infty} F[u_0] \times [\phi \operatorname{sech}^2\phi + \tanh\phi + \tanh^2\phi] \, d\phi. \tag{38}$$

The first equation determines the change in the soliton amplitude ($2\eta^2$) and width ($1/\eta$). The second of these equations gives the leading order velocity, while the last equation will give the correction to the velocity of the soliton.

From this analysis the correction u_1 is given as

$$u_1 = \int_{-\infty}^{\infty} d\lambda \, f(\lambda, t) \, \Phi^A(x, t; \lambda). \tag{39}$$

In general, for dissipative perturbations this correction will account for the development of a decaying oscillatory tail and possibly a shelf. The height of this shelf can be determined from an analysis of u_1 near $\lambda = 0$. Asymptotically, we have that [3, 4]

$$u_1 \sim \frac{1}{4\eta^3}\int_{-\infty}^{\infty} F[u_0] \tanh^2\phi \, d\phi. \tag{40}$$

A careful analysis shows that the presence of this shelf leads to the $\tanh^2\phi$ term in (38) [3, 4].

PERTURBATION ANALYSIS FOR THE ZABUSKY–KRUSKAL SCHEME

We now apply the perturbation results of the previous section to the truncation error for the Zabuskal–Krusky scheme. Using the perturbed KdV equation in (16), where

$$F[u] = -\{2u_x u_{xx} + u u_{xxx} + \tfrac{1}{4}u_{xxxxx}\}, \tag{41}$$

we evaluate (36) to find that

$$\eta_\tau = 0. \tag{42}$$

By integrating Eqs. (37) and (38) we can determine x_0 and x_1, respectively, to find that the soliton peak is located at

$$x_c = 4\eta^2 t - \tfrac{4}{5}\varepsilon\eta^4 t. \tag{43}$$

The correction to the soliton can also be determined by inserting the perturbation (41) into Eq. (39). Using the perturbation basis in Appendix A, we find that

$$u_1 = \frac{i\eta}{15}\partial_\phi \int_{-\infty}^{\infty} d\lambda \, \frac{(7\lambda^2 + 2\eta^2)(\lambda - i\eta\tanh\phi)^2}{(\lambda^2+\eta^2)\sinh(\pi\lambda/\eta)} \times [1 - e^{-8i\lambda(\lambda^2+\eta^2)t}] \, e^{-2i\lambda\phi/\eta}. \tag{44}$$

Separating the terms in the bracket under the integral and carrying out the integration we find

$$u_1 = 2\eta^4\left[-\frac{9}{10}\operatorname{sech}^2\tilde{\phi} + \frac{7}{4}\operatorname{sech}^4\tilde{\phi}\right] - \frac{i\eta}{15}\partial_\phi \int_{-\infty}^{\infty} d\lambda \, \frac{(7\lambda^2 + 2\eta^2))(\lambda + i\eta\tanh\phi)^2}{(\lambda^2+\eta^2)\sinh(\pi\lambda/\eta)} \times e^{-2i\lambda\phi/\eta - 8i\lambda(\lambda^2+\eta^2)t}, \tag{45}$$

where

$$\tilde{\phi} = \eta\,[1 - \tfrac{3}{5}\varepsilon\eta^2]\,\xi - \tfrac{1}{15}\varepsilon\eta^2, \qquad \xi = x - 4\eta^2(1 - \tfrac{1}{5}\varepsilon\eta^2)t. \tag{46}$$

From this solution we see that the first-order correction consists of additional corrections to the soliton amplitude. However, such corrections are only noticible after a sufficient amount of time has elapsed, since for small times the integral cancels the other contributions. As the soliton evolves under the perturbation, decaying oscillations develop.

According to Eq. (42), it would appear that the soliton amplitude is unaffected by the numerical scheme. However, by tracking the soliton peak in the numerical simulations, it is noticed that there is a significant effect on the soliton peak. Instead of obtaining a constant amplitude, it is found that the values of the amplitude oscillate about a constant value slightly larger that the amplitude of the initial profile, which in this case is $2\eta^2 = 2$. This behavior can be accounted for by the oscillations from the first-order correction in the above solution. This has been confirmed by comparing the numerical amplitude with that of $u_0 + \varepsilon u_1$. The order of the shift in the amplitude is $\varepsilon = \Delta x^2$.

In summary, we have found that the perturbation due to the truncation error for the Zabusky–Kruskal scheme can affect the amplitude and position, or velocity, of the soliton. Also, we do not expect to find a shelf. However, we have predicted that the most noticable effect is the shift in the center of the soliton. Previously we had defined $\varepsilon = \Delta x^2$ and from Eq. (43) we obtain the new velocity

$$v = \frac{dx_c}{dt} = 4\eta^2 - \frac{4}{5}\eta^4 \Delta x^2. \tag{47}$$

The first term is the velocity of the unperturbed soliton, and the second term is the correction due to the truncation error. Thus, we predict that the soliton is travelling at a constant velocity and is moving slower in the numerical scheme, as we had seen in Fig. 1.

A comment should be made about the validity of this perturbation analysis. Such an analysis is valid as long as the corrections remain small. From the above equation for the velocity, we see that this will be true if $\eta^2 \Delta x^2 \ll 1$. Also, we require $\varepsilon u_1/u_0 \ll 1$. Since u_1 is proportional η^4, we obtain the same condition as before. As η^{-1} is the width of the soliton, the condition, written in the form $\Delta x \ll \eta^{-1}$, says that the mesh width must be much less than the soliton width. That is, there must be a sufficient number of points across the soliton in order for the numerical scheme to provide a solution, which is close to that of the KdV equation.

We now turn to the numerical results to see how well the perturbation theory compares quantitatively to the predictions in Eqs. (42) and (43).

COMPARISON OF ANALYTICAL AND NUMERICAL RESULTS

The experiments were conducted using a wide range of values for Δx, Δt, and η. For all cases, the perturbation theory was able to accurately predict the effects of the truncation error for the Vliegenhart scheme. In a future paper, we will give an indepth report of the details of these comparisons for the Vliegenhart scheme as well as other finite difference schemes.

For clarity, we present only the case $\eta = 1$, and investigate the changes in the soliton for three values of Δx:

$$\Delta x = \tfrac{3}{8}, \tfrac{1}{4}, \tfrac{1}{8}. \tag{48}$$

The corresponding Δt's are obtained from the stability condition, which is given by Eq. (8). First, from Eq. (41) we anticipate that η will remain constant in time, but we also anticipate difficulties in measuring η, since when looking at the soliton maximum, we are measuring the soliton plus higher order corrections. To compound this problem, there is also some inaccuracy in the location of the soliton peak, due to the movement of the soliton through the spatial mesh. Having said this, we found that the soliton maximum remained constant to within 5% and the error decreased quadratically with Δx, as is to be expected from the first-order correction (45).

In Fig. 2 we display the numerical and theoretical values for the numerical shift in the soliton position for the values of Δx given above. In these studies we locate the soliton center by looking for the position at which the numerical solution reaches a maximum. These comparisons clearly show that the error in the position of the numerical soliton can be explained by the effects of the truncation error.

As a by-product of the study of this scheme, we have found that a simple modification can be made, which will increase the accuracy of the resulting simulation. Namely, we first rewrite Eq. (16) as

$$u_t + 6uu_x + u_{xxx} + \Delta x^2\{2u_x u_{xx} + uu_{xxx} + \tfrac{1}{4}u_{xxxxx}\} = 0. \tag{49}$$

This equation is then simulated by a scheme consisting of the original scheme (3)–(6) plus finite differences for u_{xx} and u_{xxxxx}, which are accurate to $O(\Delta x^2)$. In implementing such a scheme, we have found that the errors in the soliton

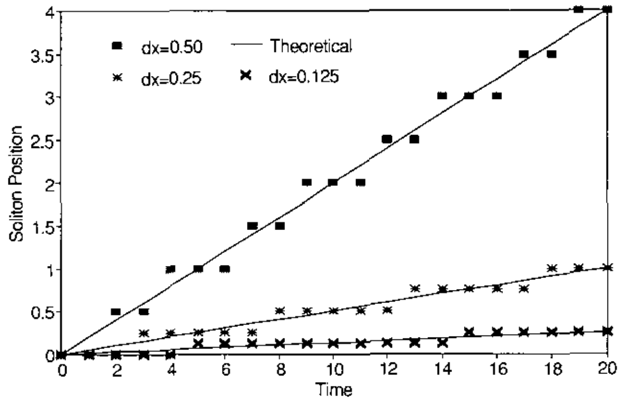

FIG. 2. Comparison of the numerical and theoretical corrections to the soliton position for $\eta = 1$, and for the three values $\Delta x = 0.375$, 0.25, 0.125.

amplitude and position are of order Δx^4, as predicted by the theory. This is a further indication of the validity of the using perturbation to study these effects.

SUMMARY

In this paper we have studied the shift in the position of the soliton in the Zabusky–Kruskal scheme. We have shown that the numerically induced phase shift can be predicted by perturbation theory.

This had been accomplished by keeping the leading order finite difference errors in the original finite difference equation, leading to a perturbed KdV equation. By studying this perturbed KdV equation we were able to obtain the leading order effects of the truncation error on the propagation of the soliton. We have found that the ZK scheme will induce a shift in the position of the soliton. As a by-product, we have suggested a simple modification of the Zabusky–Kruskal scheme, which can be implemented in about the same amount of time, but greatly reducing the errors in the amplitude and position of the soliton.

We have studied other finite difference schemes for numerically integrating both the KdV and nonlinear Schrödinger equations. Again we predict that the effects of the truncation error on the evolution of solitons can be found using singular perturbation theory. These investigations will be reported in future papers. Finally, it may also be possible that a more detailed study of the corrections to the perturbed KdV equation, which are induced by the numerical scheme, may be useful in the study of the linear stability of such schemes. We are currently looking into this problem and will report our findings at a later time.

APPENDIX A: PERTURBATION BASIS FOR A SINGLE SOLITON

In order to carry out the perturbation analysis presented in this paper, we need the following specific forms for complete set of basis states and their adjoints:

$$\Phi(x, t; \lambda) = \frac{e^{-2i\lambda\phi/\eta - 8i\lambda\eta^2 t}}{(i\lambda - \eta)^2} \times [\eta^2 \tanh^2 \phi + 2i\lambda\eta \tanh \phi - \lambda^2] \tag{A.1}$$

$$\Phi_1(x, t) = \frac{1}{4} e^{8\eta^3 t} \operatorname{sech}^2 \phi \tag{A.2}$$

$$\Lambda_1(x, t) = -\frac{i}{\eta} e^{8\eta^3 t} [(\phi + 4\eta^3 t) \operatorname{sech}^2 \phi + \tanh \phi] \tag{A.3}$$

$$\Phi^A(x, t; \lambda) = \frac{2e^{2i\lambda\phi/\eta + 8i\lambda\eta^2 t}}{(i\lambda - \eta)^2} [-\eta^3 \tanh^3 \phi + 2i\lambda\eta^2 \tanh^2 \phi + (2\lambda^2\eta + \eta^3) \tanh \phi - i(\lambda^3 + \lambda\eta^2)] \tag{A.4}$$

$$\Phi_1^A = -\frac{\eta}{2} e^{-8\eta^3 t} \operatorname{sech}^2 \phi \tanh \phi \tag{A.5}$$

$$\Lambda_1^A = 2ie^{-8\eta^3 t} \times [\operatorname{sech}^2 \phi - (\phi + 4\eta^3 t) \operatorname{sech}^2 \phi \tanh \phi] \tag{A.6}$$

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