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Davydov soliton evolution in temperature gradients driven by hyperbolic waves

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Abstract

In the present work the evolution of a Davydov soliton in an inhomogeneous medium will be considered. The Zakharov system of equations, which describes this soliton, consists of a perturbed non-linear Schrödinger (NLS) type equation plus a forced wave equation. This system is not exactly integrable for a homogeneous medium and its Lagrangian is non-local. It has recently been shown that this type of soliton has a long enough lifetime, even for non-zero temperature, so as to be a possible mechanism for the transfer of energy along an α helix. In the present work, the effect of temperature inhomogeneities on the behaviour of this soliton will be studied. As the soliton propagates through such an inhomogeneity, both dispersive and non-dispersive waves are generated. The stability of the soliton to this radiation is studied. The evolution of the Davydov soliton solution of the Zakharov equations in an inhomogeneous medium will be studied using an approximate method based on averaged conservation laws, which results in ordinary differential equations for the pulse parameters. It is shown that the inclusion of the effect of the dispersive radiation shed by the soliton for the NLS equation and the non-dispersive (hyperbolic) radiation shed by the soliton for the forced wave equation is vital for an accurate description of the evolution of the Davydov soliton. It is found that the soliton is stable even in the presence of hyperbolic radiation and that the temperature gradients have significant effects on the propagation of the soliton, even to the extent of reversing its motion.

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1. Introduction

The mechanism of energy transfer along a protein chain via the propagation of a Davydov soliton has been recently revisited [1]. In particular, the stability of the Davydov soliton under thermal fluctuations is still a matter of

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current investigation. In [2] it was shown that the Davydov soliton is stable at constant temperatures above 300 K. The problem of the influence of temperature gradients on this soliton has, however, not been considered.

The aim of the present work is to study the evolution of the Davydov soliton as it propagates into and through a temperature gradient. As the coupled Davydov soliton propagates into and through the inhomogeneous temperature, it evolves and sheds radiation. This shed radiation has two components, dispersive radiation for the NLS equation and non-dispersive (hyperbolic) radiation for the wave equation. To obtain a good description of the evolution of the Davydov soliton, the interaction between the non-dispersive radiation and the dispersive soliton must be understood. An approximate method for pulse propagation for the NLS equation was developed by [3], based on an averaged Lagrangian. By solving the linearised NLS equation, the variational equations obtained from the averaged Lagrangian were extended to include the effect of the dispersive radiation shed by an evolving pulse. However, the Zakharov equations have a non-local Lagrangian, but local conservation laws. Hence a trial function similar to that of [3] will be used in the conservation equations for the Zakharov equations to obtain approximate equations for pulse evolution, as was done by [4]. By Noether's theorem, these two methods are equivalent for a conservative system.

As in [3], the equations obtained from the conservation laws will be extended to include the effect of the radiation shed as a pulse evolves. In this regard, there is a new feature which is absent in previous radiation analyses for NLS-type equations. This new feature is that the accelerating pulse will radiate non-dispersive, hyperbolic waves in the coupled wave equation. Once proper account is made of these shed hyperbolic waves, excellent agreement is obtained between solutions of the approximate equations and full numerical solutions of the Zakharov equations. The main effect of the shed hyperbolic waves on the coupled pulses is to take away momentum so that the pulses in the NLS and wave equations can travel at the same velocity. The approximate equations are tested for extreme conditions for a perturbation theory and good quantitative agreement is found. We remark that even if the radiation in the amino-acid is of large amplitude and alters the motion of the soliton, the soliton can still act as a viable mechanism for energy transfer. The radiation mechanism found in the present work is to be expected whenever dispersive and non-dispersive waves are coupled.

This paper is organised as follows. The next, second, section summarises the known results and gives the background for the present study. The approximate Zakharov equations are then given for a Davydov soliton in a temperature gradient. The third section derives the approximate equations from conservation laws, while the fourth section extends these approximate equations to include the effect of the shed radiation, with the fifth section comparing solutions of the approximate equations with full numerical solutions of the Zakharov equations. Finally, the last section presents conclusions.

2. Formulation

The Davydov equations describe the collective motion of a protein chain [5]. In this model the protein chain is idealised as a discrete chain with peptide groups at each site of the chain. These peptide groups are in turn linked together by amino-acids with the peptide groups described in terms of their quantum excitations. The model then couples the quantum compressional motion of the amino-acids to the peptide groups by the exchange of phonons which can excite transitions in the peptides and vice versa. The quantum mechanics of this model system was formulated by Davydov [5]. A simple, modern formulation is given in [6].

In [5,6] the variables $a_n(t)$ denote the probability of finding one quantum of excitation in the peptide at site n. These variables are normalised so that

$$\sum_{n=-\infty}^{\infty} |a_n|^2 = 1. \tag{1}$$

The variables $\beta_n(t)$ are then the quantum mechanical average for the displacement of the amino-acid at site n. Schrödinger's equation for the system [5] then gives the equations of motion for these variables in the form

$$\hbar \dot{a}_n = -\mathcal{J}(a_{n+1} + a_{n-1}) + \chi(\beta_{n+1} - \beta_{n-1})a_n, \tag{2}$$

$$m\ddot{\beta}_n = w(\beta_{n+1} - 2\beta_n + \beta_{n-1}) + \chi(|a_{n+1}|^2 - |a_{n-1}|^2). \tag{3}$$

In these equations $\mathcal{J}$ is a measure of the dipole–dipole interaction, w is the restoring force in the molecular chain, m the mass of the amino-acid and χ is a measure of the effectiveness of energy transfer from one peptide group to another, analogous to a susceptibility [5,6]. In the continuum limit these equations become the Davydov equations, which are, with the change of variables $a_n \to \varphi$ and $\beta_n \to \beta$,

$$\mathrm{i}\hbar \frac{\partial \varphi}{\partial t} = -\mathcal{J}\frac{\partial^2 \varphi}{\partial x^2} + 2\chi\varphi\frac{\partial \beta}{\partial x}, \tag{4}$$

$$m\frac{\partial^2 \beta}{\partial t^2} - w\frac{\partial^2 \beta}{\partial x^2} = 2\chi\frac{\partial}{\partial x}|\varphi|^2. \tag{5}$$

It is now convenient to introduce the new variable

$$\eta = \frac{\partial \beta}{\partial x} \tag{6}$$

and to obtain the amino-acid displacement in the form

$$\beta(x) = -\int_x^\infty \eta \, \mathrm{d}\xi. \tag{7}$$

With these new variables the Davydov equations are the same as the Zakharov equations for the interaction of a wave packet with non-dispersive radiation governed by the wave equation for η.

A problem which has been studied is the stability of the Davydov soliton under temperature fluctuations. There are two different approaches to this. In the first approach a random force of Langevin type is added to Eq. (5) for β. It was shown by [7] that for temperatures of the order 10 K the soliton is unstable since it decays very rapidly as compared with the minimum time required to transport energy along the chain.

The second approach is to use the appropriate quantum mechanical statistical average [5,8]. In this approach the thermal motion of the phonons is shown to screen, with the Debye factor, the strength of the long-range dipole–dipole interactions. This screening results in a modification of $\mathcal{J}$ in Eq. (4) for φ. It was shown in [5,8] that $\mathcal{J}$ becomes a functional of the displacements β_n. It was further shown that the decrease in $\mathcal{J}$ due to screening results in the soliton being stable for temperatures above 300 K. The study of [5] assumed the adiabatic approximation

$$\frac{\partial^2 \beta}{\partial t^2} \approx 0 \tag{8}$$

and also assumed that the screened $\mathcal{J}$ was independent of position. However, this study did not include the waves which may be emitted by the soliton as it evolves. Another study [8] took into account the non-adiabatic motion of the amino-acids and included the dependence of the screening on the displacements β_n. Again it was found that solitons are stable for temperatures above 300 K.

In the present work a complementary point of view is taken. As in [8] the motion will be taken to be non-adiabatic and as in [5] it will be assumed that the screening does not depend on β. However, it will be assumed that the temperature is inhomogeneous and is slowly varying along the chain. The effect of a temperature gradient on a soliton will then be studied. In this work, we take, as in [5], the equations for the peptides in the form:

$$\mathrm{i}\hbar \frac{\partial \varphi}{\partial t} + \frac{\hbar^2}{M}\,\mathrm{e}^{-W}\frac{\partial^2 \varphi}{\partial x^2} - 2\mathcal{J}(1 - \mathrm{e}^{-W})\varphi + G|\varphi|^2\varphi = 0, \tag{9}$$

where $1-\exp(-W)$ is the effect of the phonon vibrations which produce the screening of the dipole–dipole interactions, the constant G is the effect of the coupling of the motion of the chain with sound waves in the adiabatic approximation and M is the mass of the peptide [5,6].

In the non-adiabatic approximation the equations governing the protein chain are (4) and (5) with the screened $\mathcal{J}$ given as in Eq. (9). In normalised variables, Eqs. (4) and (5) take the forms

$$\mathrm{i}\frac{\partial\varphi}{\partial t}+\frac{1}{2}\frac{\partial^2\varphi}{\partial x^2}-2\mathcal{J}(1-\mathrm{e}^{-W})\varphi+\eta\varphi=0, \tag{10}$$

$$\frac{\partial^2\beta}{\partial t^2}-\frac{\partial^2\beta}{\partial x^2}=\frac{\partial^2}{\partial x^2}|\varphi|^2. \tag{11}$$

In the present work, the term $2\mathcal{J}(1-\mathrm{e}^{-W})$ is assumed to be slowly varying along the protein chain.

In order to understand the effect of temperature gradients on a soliton, the Zakharov system of Eqs. (10) and (11) for the chain will be taken in the form

$$\mathrm{i}\frac{\partial E}{\partial t}+\frac{1}{2}\frac{\partial^2 E}{\partial x^2}-\eta E+f(x)E=0,\quad -\infty<x<\infty,\quad t\geq 0, \tag{12}$$

$$\frac{\partial^2\eta}{\partial t^2}-\frac{\partial^2\eta}{\partial x^2}=\frac{\partial^2}{\partial x^2}|E|^2 \tag{13}$$

on changing φ to E in order to conform with the usual notation for the Zakharov equations. The first of these Zakharov equations is a perturbed non-linear Schrödinger (NLS) equation, while the second is a forced wave equation. In the protein chain context, $f(x)$ accounts for a localised thermal effect. For f constant, the Zakharov equations has the Davydov soliton solution

$$E=a\,\mathrm{sech}\left(a\frac{x-Vt}{\sqrt{1-V^2}}\right)\mathrm{e}^{\mathrm{i}[(1/2)(a^2/(1-V^2))t+V(x-(1/2)Vt)+ft]}, \tag{14}$$

$$\eta=-\frac{a^2}{1-V^2}\mathrm{sech}^2\left(a\frac{x-Vt}{\sqrt{1-V^2}}\right). \tag{15}$$

The object of the present work is to determine the effect of changing medium on this Davydov soliton, so that f changes.

It is well established that on keeping $\eta=-|E|^2/(1-V^2)$ even in the non-uniform region, the soliton accelerates or decelerates as it enters the region of non-uniform medium described by $f(x)$. However, when the effect of the wave equation (13) is included, a new feature appears. From the wave equation it can be seen that as $|E|$ changes in the non-uniform region, a substantial amount of radiation in η will be produced in addition to the already present soliton (15) in η. This radiation will be found to have an influence on the motion of the soliton in both the E and η modes. This influence of radiation is missed if only the NLS equation is considered by keeping $\eta=-|E|^2/(1-V^2)$. In particular, the question of the persistence of the soliton is decided by the shed radiation. Therefore, proper account of the shed radiation is needed in order to study the effect of non-uniform temperature on the soliton.

Thus the aim of the present work is to study the influence of the non-dispersive radiation shed by the Davydov soliton as it propagates in and through the region of non-uniform media, this radiation being governed by the wave equation (13). The effect of this radiation on the evolution of the Davydov soliton will be determined using an approximate method based on that of [3]. This approximate method is based on the use of an averaged Lagrangian. While the Zakharov equations (12) and (13) do not possess a local Lagrangian, they do possess a non-local Lagrangian which can be obtained via changing the dependent variables as

$$u=\int_0^t(\eta+|E|^2)\,\mathrm{d}t, \tag{16}$$

which results in the transformed equations

$$\mathrm{i}\frac{\partial E}{\partial t} + \frac{1}{2}\frac{\partial^2 E}{\partial x^2} - E\frac{\partial u}{\partial t} + |E|^2 E + f(x)E = 0, \tag{17}$$

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial t}|E|^2. \tag{18}$$

It should be noted that the variable u is an artifical variable and is not the physical amino-acid displacement. This coupled set of equations in the variables u and E has the Lagrangian

$$L = \iint [\mathrm{i}(E^* E_t - E E_t^*) - |E_x|^2 + |E|^4 + u_t^2 - u_x^2 - 2|E|^2 u_t + f(x)|E|^2]\,\mathrm{d}x\,\mathrm{d}t. \tag{19}$$

This Lagrangian (19) could now be used to derive approximate equations for the evolution of a Davydov soliton following the work of [3]. However, the transformation (16) leads to non-local equations for the parameters of the modulated soliton, which are not a suitable set of approximate equations to study its evolution. Therefore in the next section, we shall use the basic conservation equations for the Zakharov equations (12) and (13) to obtain equations for these parameters. On the other hand, the Lagrangian (19) does indicate the appropriate conservation equations to use since it is clear from this Lagrangian that conservation of momentum includes the soliton in both the NLS and wave equations and the generated radiation and not each equation separately.

3. Approximate equations

We shall now seek an approximate solution of the Zakharov equations (12) and (13) based on the method of [3]. We therefore seek approximate solutions in the form

$$E = a\,\mathrm{sech}\left(\frac{x-y}{w}\right)\mathrm{e}^{\mathrm{i}[\sigma + V(x-y)]} + \mathrm{i}g\,\mathrm{e}^{\mathrm{i}[\sigma + V(x-y)]}, \tag{20}$$

$$\eta = -A\,\mathrm{sech}^2\left(\frac{x-y}{w}\right). \tag{21}$$

In these trial solutions, the amplitudes a and A, width w, position y, velocity V, phase σ and g are functions of time t. The first term in (20) and the trial function (21) are varying soliton-like pulses, as can be seen on comparing with the soliton solutions (14) and (15). The second term in the trial solution (20) for E represents the low frequency dispersive radiation in the vicinity of the pulse E [3]. As the pulse in E evolves, it sheds dispersive radiation in order to reach a steady state. That this radiation in the vicinity of the pulse is independent of x can be seen from the following group velocity argument. The dispersion relation for linear waves for the NLS equation (12) for $f = 0$ is $\omega = k^2/2$, where ω is the frequency of the waves and k is the wavenumber. Hence the group velocity of these waves is $c_\mathrm{g} = k$, so that low wavenumber waves have low group velocity relative to the pulse and so stay with the evolving pulse. This shelf of radiation under the E pulse is represented by g. As the shed dispersive radiation has small amplitude relative to the pulse, $|g| \ll a$. The dispersive radiation cannot, of course, remain independent of x away from the vicinity of the pulse. Hence, as in [3], it is assumed that the shed radiation is flat in the region $y - \ell/2 \le x \le y + \ell/2$ around the pulse and g is taken to be zero outside of this region. The form of the radiation outside of this region will be considered in the next section. As the wave equation (13) is non-dispersive, the phase and group velocities for any shed waves are 1, so that there is no shelf of radiation under the pulse in η. We remark that the term g is also present for the homogeneous case $f = 0$ since initial conditions which are not exact solitons always shed low wavenumber radiation in order to evolve to a soliton state [3].

The initial condition to be used in the present work is the Davydov soliton solution (14) and (15). The Davydov soliton starts at $x = 0$ with amplitude $a = a_0$ and velocity $V = V_0$. Therefore, the initial values of the parameters in the trial solutions (20) and (21) are

$$a = a_0, \qquad w = \frac{\sqrt{1 - V_0^2}}{a_0}, \qquad V = V_0, \qquad y = 0 \quad \text{and} \quad g = 0. \tag{22}$$

Before proceeding to the approximate equations derived from the trial functions (20) and (21), let us derive a qualitative description for evolution of the pulses on assuming that all of the parameters in the trial functions are constant, except for y and $V = \dot{y}$, and that $g = 0$, so that any shed dispersive radiation is neglected. Let us also assume that a, A and w are related as for the Davydov soliton (14) and (15) with $f = 0$, so that $w = \sqrt{1 - V^2}/a$ and $A = a^2/(1 - V^2)$. Substituting these restricted trial functions into the Lagrangian (19), we derive the averaged Lagrangian by integrating in x from $x = -\infty$ to ∞. Taking the variational equation in y for this averaged Lagrangian gives the equation for the soliton position as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\left(a^2 w + \frac{a^4 w}{(1 - V^2)^2}\right) V\right] - \frac{\partial \phi}{\partial y} = 0, \tag{23}$$

where the potential $\phi(y)$ is

$$\phi = \int_{-\infty}^{\infty} f(x) \operatorname{sech}^2 \frac{x - y}{w}\, \mathrm{d}x. \tag{24}$$

The details of the motions of the pulses depends on the detailed form of $f(x)$. Let us therefore consider the special case

$$f(x) = \begin{cases} 0 & x \le 0, \\ mx & 0 < x \le L, \\ mL & x > L. \end{cases} \tag{25}$$

This form for f represents the left-hand end of the chain at room temperature and the right-hand end $x = L$ at the temperature mL. In this case, the potential (24) is given by

$$\phi(y) = wmL - mw^2 \log\left(\frac{\cosh\left[(L - y)/w\right]}{\cosh\left(y/w\right)}\right), \tag{26}$$

which is a monotonic function. Based on this potential, we have two possible motions. When the potential is decreasing, the soliton accelerates and leaves the inhomogeneous region with changed velocity. On the other hand, when the potential is increasing and the initial energy is lower than the maximum potential barrier, the soliton will partly penetrate the inhomogeneous region and then bounce back. For the potential (26) there is no possibility that the soliton will stop in the inhomogeneous region, as the potential is monotone.

Other forms of the inhomogeneity $f(x)$ will lead to different trajectories of the soliton. For example, if

$$f(x) = \alpha(x - x_1)^2 \tag{27}$$

the soliton will oscillate in the inhomogeneous region and eventually settle onto a steady state with zero velocity due to the shedding of radiation.

Let us now return to the general trial functions (20) and (21) for which all the parameters are functions of time t. The ordinary differential equations governing these parameters will be derived from conservation equations for the Zakharov equations (12) and (13). The NLS equation (12) possesses the mass and energy conservation equations:

$$\mathrm{i}\frac{\partial}{\partial t}|E|^2 + \frac{1}{2}\frac{\partial}{\partial x}(E^* E_x - E E_x^*) = 0, \tag{28}$$

$$\mathrm{i}\frac{\partial}{\partial t}(|E_x|^2 - 2f|E|^2 + 2\eta|E|^2) + \frac{1}{2}\frac{\partial}{\partial x}[E_x^* E_{xx} - E_x E_{xx}^* + 2(\eta - f)(E^* E_x - E E_x^*)] = 2\mathrm{i}|E|^2\frac{\partial \eta}{\partial t} \tag{29}$$

and the moment of momentum equation

$$\begin{aligned}\mathrm{i}\frac{\partial}{\partial t}[x(E^* E_x - E E_x^*)] &+ \frac{1}{2}\frac{\partial}{\partial x}[x(E^* E_{xx} + E E_{xx}^*) - 2x|E_x|^2 - E^* E_x - E E_x^*] \\ &= 2x|E|^2\frac{\partial \eta}{\partial x} - 2x|E|^2 f' - 2|E_x|^2,\end{aligned} \tag{30}$$

where the superscript * denotes the complex conjugate. In addition, the wave equation (13) possesses the mass conservation equation

$$\frac{\partial}{\partial t}\left(\frac{\partial \eta}{\partial t}\right) - \frac{\partial}{\partial x}\left(\frac{\partial \eta}{\partial x} + \frac{\partial}{\partial x}|E|^2\right) = 0. \tag{31}$$

Finally, the NLS equation (12) and the wave equation (13) possess the total momentum conservation equation

$$\begin{aligned}\frac{\partial}{\partial t}[\mathrm{i}(E^* E_x - E E_x^*) + \eta_x \eta_t] &+ \frac{1}{2}\frac{\partial}{\partial x}[E^* E_{xx} + E E_{xx}^* - 2|E_x|^2 - \eta_t^2 - \eta_x^2] \\ &= 2|E|^2\frac{\partial \eta}{\partial x} - 2|E|^2 f' + \frac{\partial \eta}{\partial x}\frac{\partial^2}{\partial x^2}|E|^2.\end{aligned} \tag{32}$$

For the form of the inhomogeneity, let us take a slight generalisation of the linear form (25)

$$f(x) = \begin{cases} f_1 & x \le x_1, \\ m(x - x_1) + f_1 & x_1 < x \le x_2, \\ f_2 & x > x_2, \end{cases} \tag{33}$$

where

$$m = \frac{f_2 - f_1}{x_2 - x_1}. \tag{34}$$

This profile for f is just a linear gradient with level f_1 in $x \le x_1$ going to the level f_2 at $x = x_2$ and represents an arbitrary linear temperature gradient.

Substituting the trial functions (20) and (21) into the conservation and moment equations (28)–(32), we obtain, after some algebra,

$$\frac{\mathrm{d}}{\mathrm{d}t}(\eta w) = \frac{\ell g}{2\pi}\left[2A - w^{-2} - m(x_2 - y)\tanh\frac{x_2 - y}{w} + m(x_1 - y)\tanh\frac{x_1 - y}{w} + f_1 + f_2\right], \tag{35}$$

$$\begin{aligned}\pi a w\frac{\mathrm{d}g}{\mathrm{d}t} = \frac{2a^2}{3w}(1 - Aw^2) &+ ma^2 w\left[(x_2 - y)\tanh\frac{x_2 - y}{w} - (x_1 - y)\tanh\frac{x_1 - y}{w}\right] \\ &- ma^2 w^2 \log\left[\frac{\cosh(x_2 - y)}{\cosh(x_1 - y)}\right],\end{aligned} \tag{36}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{a^2}{w} - 4Aa^2 w\right) = -4a^2 w\frac{\mathrm{d}A}{\mathrm{d}t} - 2Aa^2\frac{\mathrm{d}w}{\mathrm{d}t}, \tag{37}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(Aw) = 0, \tag{38}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[(2a^2w+\ell g^2)V+\frac{A^2V}{w}\right]=ma^2w\left(\tanh\frac{x_2-y}{w}-\tanh\frac{x_1-y}{w}\right), \tag{39}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t}=V. \tag{40}$$

Eq. (37) is the equation for conservation of energy for the pulse for the NLS equation, Eq. (38) is the equation for mass conservation for the pulse for the wave equation, on assuming that $(Aw)'=0$ initially, and Eq. (39) is the equation for total momentum conservation. On combining equations (35)–(37), the mass conservation equation for the pulse for the NLS equation can be obtained

$$\frac{\mathrm{d}}{\mathrm{d}t}(2a^2w+\ell g^2)=0. \tag{41}$$

The final parameter to be determined is the length ℓ of the shelf under the pulse for the NLS equation. This parameter was determined by [3] by requiring that the frequency of oscillation of the solution of the approximate equations for the pulse evolution near the fixed point matches the NLS soliton oscillation frequency. Linearising the approximate equations (35)–(40) about the soliton fixed point

$$w=\frac{\sqrt{1-V^2}}{a},\qquad A=\frac{a^2}{1-V^2},\quad f=\text{constant},\quad V=\text{constant} \tag{42}$$

gives

$$\ell=\frac{3\pi^2\sqrt{1-V^2}}{8\hat{a}} \tag{43}$$

on noting from the soliton solution (14) that the soliton oscillation frequency is

$$\frac{\hat{a}^2}{2(1-V^2)}. \tag{44}$$

The value $\hat{a}$ is the fixed point value of the NLS soliton amplitude. For constant $f(x)$, this fixed point value can be determined from the energy conservation equation (37). However, when $f(x)$ is not constant this cannot be done. Hence the values of a and V in the expression (43) for ℓ are taken to be their local values at t rather than their fixed point values, as was done by [9].

The system of ordinary differential equations (35)–(40) is not yet complete as the effects of the dispersive radiation shed by the pulse for the NLS equation and the non-dispersive radiation shed by the pulse for the wave equation have not been included. The effect of these two components of the shed radiation will be considered in the next section.

4. Radiation loss

The dispersive radiation shed by the pulse in the NLS equation has small amplitude. Therefore, away from the pulse, this radiation is governed by the linearised NLS equation

$$\mathrm{i}\frac{\partial E}{\partial t}+\frac{1}{2}\frac{\partial^2E}{\partial x^2}+f(x)E=0. \tag{45}$$

For general $f(x)$, this linearised equation does not have an exact solution. However, if $f(x)$ is taken to be slowly varying, then to first order, the transformation

$$E=U\,\mathrm{e}^{\mathrm{i}ft} \tag{46}$$

results in the linearised NLS equation

$$\mathrm{i}\frac{\partial U}{\partial t} + \frac{1}{2}\frac{\partial^2 U}{\partial x^2} = 0. \tag{47}$$

This is the same linearised NLS equation that was considered by [3] to determine the effect of shed dispersive radiation on the evolution of a soliton-like pulse for the NLS equation. Therefore, full details of the calculation of the effect of this radiation will not be given here, only a brief outline, with the full details given in [3].

From the linearised NLS equation (47), it can be shown that the mass shed to the right of the pulse as dispersive radiation is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{y+\ell/2}^{\infty} |U|^2\,\mathrm{d}x = \mathrm{Im}(U^* U_x)|_{x=y+\ell/2}. \tag{48}$$

For constant V, this is the same as the mass shed in dispersive radiation to the left of the pulse. On solving the linearised NLS equation (47) using Laplace transforms, U_x can be related to U via the convolution integral

$$U_x\left(y+\frac{\ell}{2}, t\right) = -\sqrt{2}\,\mathrm{e}^{-\mathrm{i}\pi/4}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{U(y+\ell/2,\tau)}{\sqrt{\pi(t-\tau)}}\,\mathrm{d}\tau. \tag{49}$$

This relation between U_x and U has been derived under the assumption that V is constant. If V is not constant, then determining the mass flux from the evolving pulse would involve a moving boundary value problem with the moving boundary, the edge of the shelf under the pulse, unknown and determined by the solution of the approximate equations of the previous section. However, if the inhomogeneous region is slowly varying, then V will be slowly varying and so can be taken to be constant to first order.

The mass loss expression (48), and a symmetric one for mass loss to the left of the pulse, can now be added to the conservation of mass equation for the pulse (41) to give the new mass conservation equation for the pulse which takes account of mass loss to dispersive radiation

$$\frac{\mathrm{d}}{\mathrm{d}t}(2a^2 w + \ell g^2) = 2\sqrt{2}\,\mathrm{Im}\left[\mathrm{e}^{-\mathrm{i}\pi/4} u^*\left(y+\frac{\ell}{2}, t\right)\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{u(y+\ell/2,\tau)}{\sqrt{\pi(t-\tau)}}\,\mathrm{d}\tau\right]. \tag{50}$$

It was noted in [3] that the phase of $u(y+\ell/2, t)$ is slowly varying since the shelf is small in magnitude and flat. Hence both u and u^* in (50) can be replaced by $r = |u(y+\ell/2, t)|$, so that the mass conservation equation (50) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}(2a^2 w + \ell g^2) = -2r(t)\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{r(\tau)}{\sqrt{\pi(t-\tau)}}\,\mathrm{d}\tau. \tag{51}$$

By linearising the mass conservation equation (41) about the soliton fixed point (42) it is found that

$$r^2 = \frac{3a}{8\sqrt{1-V^2}}\left[2a^2 w - 2a\sqrt{1-V^2} + \ell g^2\right] \tag{52}$$

as in [3].

When the mass loss in (51) is added to the approximate equations (35)–(40), Eq. (36) for g becomes

$$\begin{aligned}\pi a w\frac{\mathrm{d}g}{\mathrm{d}t} = {} & \frac{2a^2}{3w}(1-Aw^2) + ma^2 w\left[(x_2-y)\tanh\frac{x_2-y}{w} - (x_1-y)\tanh\frac{x_1-y}{w}\right] \\ & - ma^2 w^2 \log\left[\frac{\cosh(x_2-y)}{\cosh(x_1-y)}\right] - 2\alpha\pi a w g.\end{aligned} \tag{53}$$

The loss coefficient α is

$$\alpha = \frac{3a}{8\sqrt{1-V^2}}\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{r(\tau)}{\sqrt{\pi(t-\tau)}}\,\mathrm{d}\tau. \tag{54}$$

The system of approximate equations governing the evolution of the pulses for the Zakharov equations, including dispersive radiation shed by the NLS pulse, is then (35), (37)–(40) and (53).

Now that the effect of the radiation shed by the pulse in the NLS equation has been calculated, we need to determine the effect of the non-dispersive radiation shed by the pulse in the wave equation (13). The form of this shed non-dispersive radiation can be seen in Fig. 1(a) which shows the full numerical solution of the Zakharov equations (12) and (13) for a monotonic decreasing potential with $x_1 = 8$, $x_2 = 9$, $f_1 = 0$ and $f_2 = 0.1$. The details of the numerical method used to obtain this solution will be given in the next section. The Davydov soliton accelerates through the inhomogeneous region and emerges with a larger velocity and higher amplitude. Figs. 1(b) and (c) show comparisons between the full numerical solution and the solution of the approximate equations (35), (37)–(40) and (53) for the amplitude of the E pulse and the velocity of the pulses V. It can be seen that the agreement between the approximate and numerical solutions is not good. The reason for this difference can be seen from Fig. 1(a). It can be seen from this figure that there is a relatively large lump of radiation in the amino-acid displacement wave η lying ahead of the main pulse, which moves with the NLS soliton. It is this shed non-dispersive (hyperbolic) radiation which must be taken into account in the approximate equations.

On examining the trial function (21) for the amino-acid displacement wave η, we note that it does not take account of any non-dispersive radiation shed by the η pulse as it evolves. We therefore need to modify the approximate equations for η take account of the shed wave seen in Fig. 1(a). To find the form of this shed wave, we integrate the wave equation (13) for a given $|E|^2$ using the D'Alembert solution to obtain

$$\eta(x,t) = \frac{1}{2}[\eta_0(x-t)+\eta_0(x+t)] + \frac{1}{2}\int_{x-t}^{x+t} v(\xi)\,\mathrm{d}\xi + \frac{1}{2}\int_0^t\int_{x-(t-\tau)}^{x+(t-\tau)} |E|^2_{\xi\xi}(\xi,\tau)\,\mathrm{d}\xi\,\mathrm{d}\tau, \tag{55}$$

where the initial conditions for η are $\eta(x,0) = \eta_0(x)$ and $\eta_t(x,0) = v(x)$. Given $|E|$, this is an exact solution for η. However, $|E|$ is not known, so we use the trial function (20) for E instead.

Since the initial condition is the Davydov soliton (14) and (15), the initial conditions η_0 and v in the D'Alembert solution can be explicitly calculated. Then using the trial function (20) for E, integrating the D'Alembert solution (55) by parts gives

$$\eta(x,t) = -\frac{a^2}{1-V^2}\mathrm{sech}^2\left(\frac{x-y}{w}\right) - \frac{1}{2}\int_0^t \left[a^2\mathrm{sech}^2\left(\frac{x-y(\tau)+t-\tau}{w}\right)\frac{\mathrm{d}}{\mathrm{d}\tau}\frac{1}{1+V(\tau)} + a^2\mathrm{sech}^2\left(\frac{x-y(\tau)-(t-\tau)}{w}\right)\frac{\mathrm{d}}{\mathrm{d}\tau}\frac{1}{1-V(\tau)}\right]\mathrm{d}\tau. \tag{56}$$

For constant velocity V, this expression for η is exactly the Davydov soliton (15). Notice that the extra term in (56) comes from the waves radiated due to the pulse acceleration. Now the fixed point of the approximate equations (35)–(40) has

$$A = \frac{a^2}{1-V^2}. \tag{57}$$

To be consistent with the trial function (21), let us therefore replace $a^2/(1-V^2)$ in (56) by A, which is valid in the limit of slowly varying V.

Now integrating the wave equation (13) gives the mass conservation equation

$$\int_{-\infty}^{\infty}\eta(x,t)\,\mathrm{d}x = \int_{-\infty}^{\infty}\eta(x,0)\,\mathrm{d}x = 2A(0)w(0) \tag{58}$$

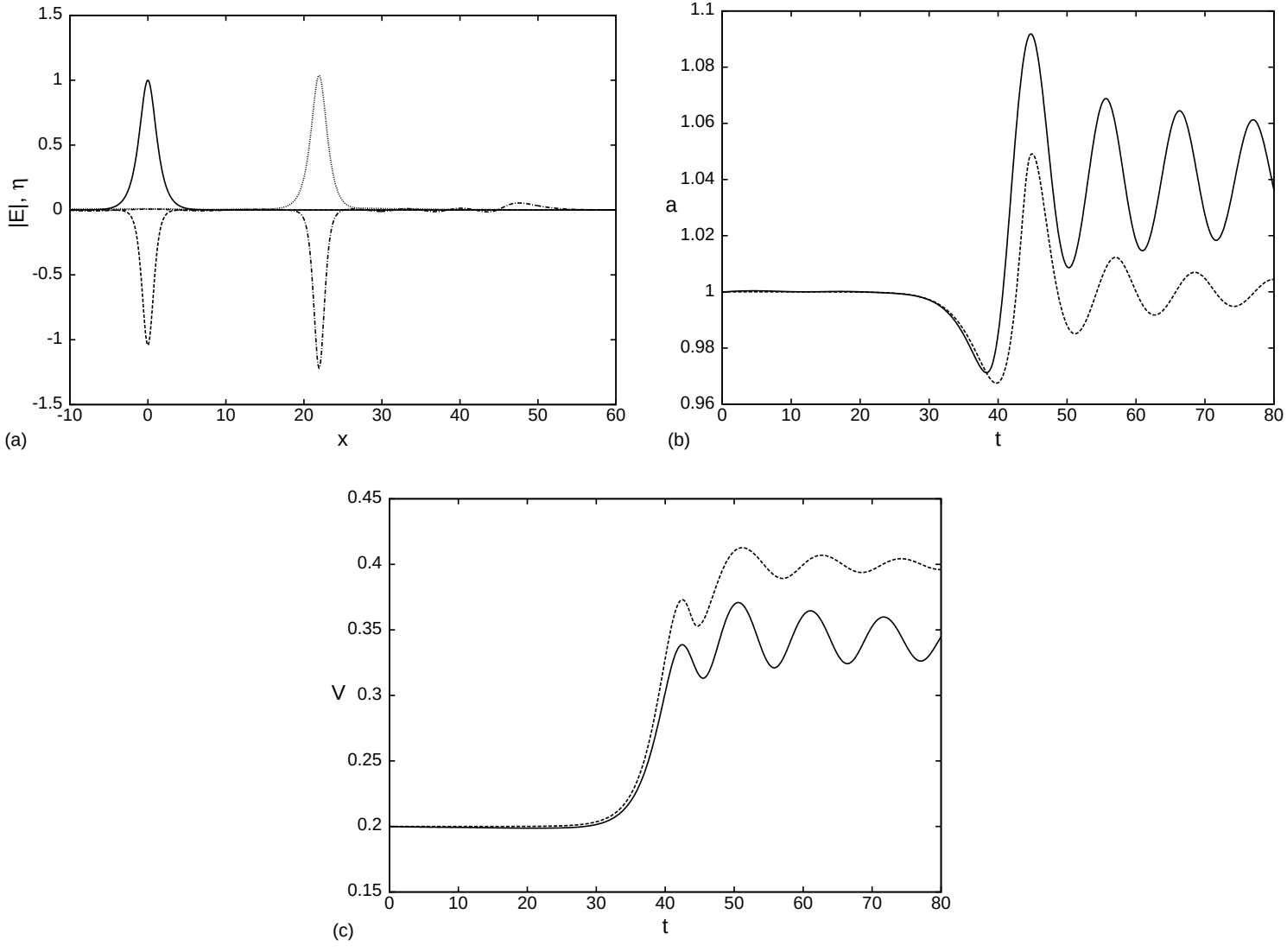

Fig. 1. Full numerical and approximate solutions of the Zakharov equations (12) and (13) for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.2$ for $x_1 = 8$, $x_2 = 9$, $f_1 = 0$ and $f_2 = 0.1$. (a) (—) initial condition for $|E|$; (– – –) initial condition for η; (- - -) solution for $|E|$ at $t = 80$; (– – –) solution for η at $t = 80$. (b) Amplitude of electric field $|E|$: (—) full numerical solution; (– – –) solution of approximate equations (35), (37)–(40) and (53) (without non-dispersive radiation loss). (c) Velocity of pulses V: (—) full numerical solution; (– – –) solution of approximate equations (35), (37)–(40) and (53) (without non-dispersive radiation loss).

for the wave equation. Substituting the D'Alembert expression for η (56) into this mass conservation equation, we obtain

$$A(t) = \frac{A(0)w(0)}{w(t)} + \frac{2}{w(t)} \int_0^t \frac{a^2(\tau)w(\tau)V(\tau)\dot{V}(\tau)}{(1 - V^2(\tau))^2}\, \mathrm{d}\tau. \tag{59}$$

This mass conservation equation replaces the mass conservation equation (38) of the approximate equations of the previous section. The mass shed as non-dispersive (hyperbolic) radiation by the pulse in the wave equation, which is due to the acceleration of the pulse, is given by the integral term in (59).

The full set of approximate equations governing the evolution of the Davydov soliton, including the effects of shed dispersive and non-dispersive radiation, is then (35), (37), (39), (40), (53) and (59). If the effect of the shed non-dispersive radiation is not included, the approximate equations are then (35), (37)–(40) and (53).

5. Results

In this section, full numerical solutions of the Zakharov equations (12) and (13) will be compared with numerical solutions of the approximate equations. Numerical solutions of the NLS equation (12) were obtained using a pseudo-spectral method based on that of Fornberg and Whitham [10]. This method involves calculating the dispersive and non-linear terms in the NLS equation using fast Fourier transforms (FFTs) and then propagating the resulting ode forward in time t in Fourier space using a fourth-order Runge–Kutta method. The wave equation (13) was solved using standard second-order finite differences with the forcing term $|E|_{xx}$ calculated using FFTs. Finally, the approximate equations were solved numerically using a fourth-order Runge–Kutta method, with the integral in the loss coefficient (54) calculated using the trapezoidal rule based method of [11] which deals with the singularity at $t = \tau$.

Let us first consider the case of increasing inhomogeneity, in which case the soliton passes through it. As a first example, let us return to the example shown in Fig. 1, which in the previous section was used to suggest the importance of the shed hyperbolic radiation. The inhomogeneity extends from $x_1 = 8$ to $x_2 = 9$ and has a small jump of 0.1. The length of the inhomogeneity is comparable to the width of the soliton, and so appears as an abrupt jump to it. It can be seen from Fig. 2(a) that including the effect of the shed non-dispersive radiation results in much improved agreement with the full numerical solution for the soliton amplitude a, particularly in the mean of the amplitude oscillations. However, the damping effect of the calculated non-dispersive radiation loss is too great and the amplitude oscillations are damped at too great a rate as compared with the full numerical solution. Fig. 2(b) and (c) show comparisons between the full numerical and approximate solutions for the wave pulse amplitude A and the pulse velocity V, respectively. Again, including the non-dispersive radiation loss results in excellent agreement in the mean, but results in too rapid a damping of the amplitude and velocity oscillations.

Fig. 3 shows comparisons between the full numerical solution of the Zakharov equations and the solution of the approximate equations for a jump of height 0.1 extending from $x_1 = 1$ to $x_2 = 2$. As the Davydov soliton starts at $x = 0$, there is some overlap of the forward tail of the soliton into the inhomogeneous region. The length of the inhomogeneous region is again comparable to the width of the soliton. Fig. 3(a) and (b) show comparisons of the full numerical and approximate solutions for the NLS pulse amplitude a and the wave equation pulse amplitude A, respectively. There is reasonable agreement between the full numerical solution and the solution of the approximate equations with non-dispersive radiation loss, with again the damping of the amplitude oscillations in the approximate solution being too great. However, the inclusion of the effect of the non-dispersive radiation loss is needed in order to obtain agreement with the full numerical solution, with the solution without non-dispersive radiation loss oscillating about the initial amplitude. Fig. 3(c) shows the comparison for the pulse velocity V. The effect of the inclusion of

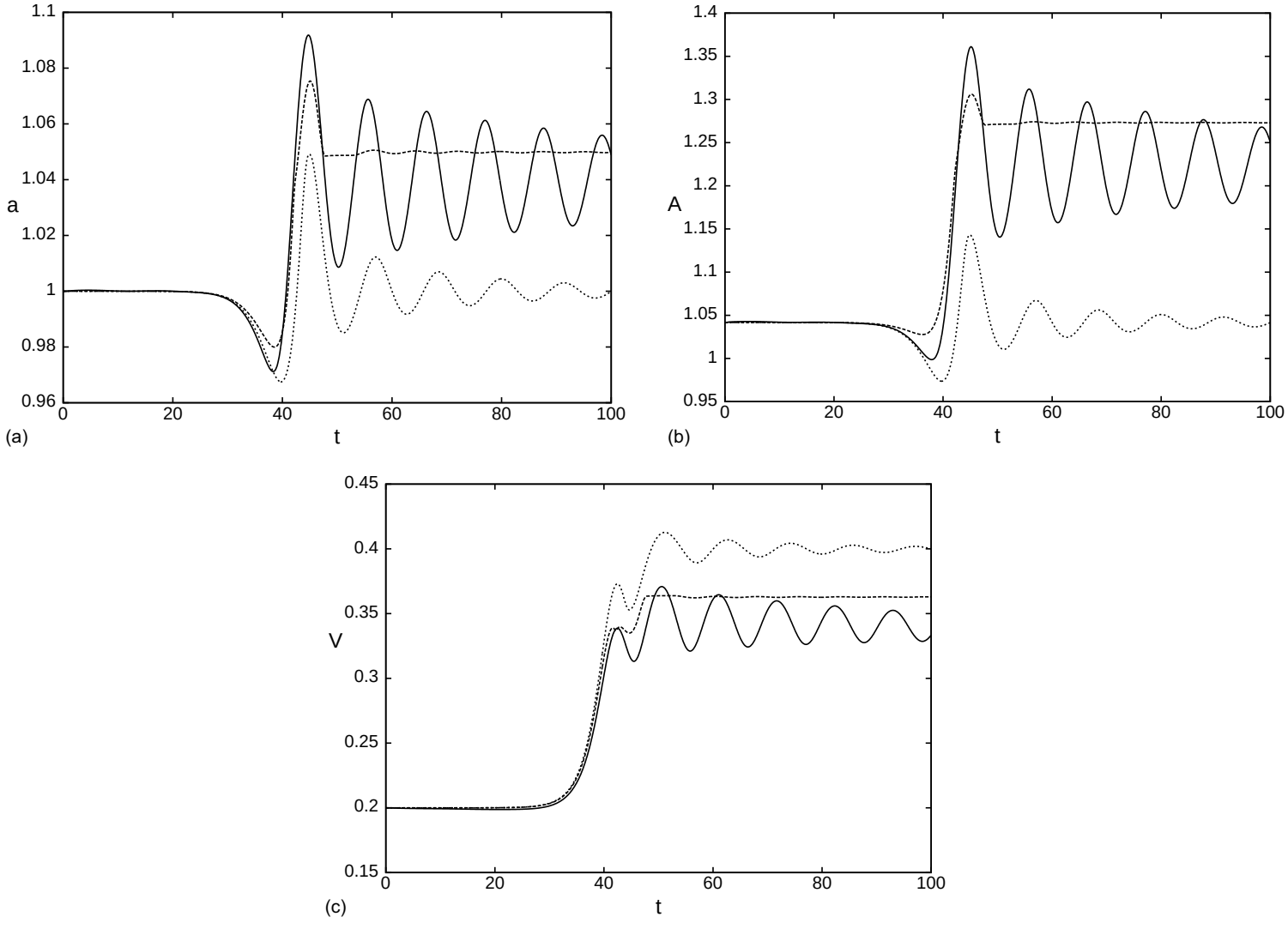

Fig. 2. Comparison between full numerical solution of Zakharov equations and solution of approximate equations for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.2$ for $x_1 = 8$, $x_2 = 9$, $f_1 = 0$ and $f_2 = 0.1$. (—) full numerical solution; (– – –) solution of approximate equations with loss to non-dispersive radiation; (- - -) solution of approximate equations with no loss to non-dispersive radiation. (a) Amplitude a of NLS soliton, (b) amplitude A of soliton in wave equation and (c) velocity V of the pulses.

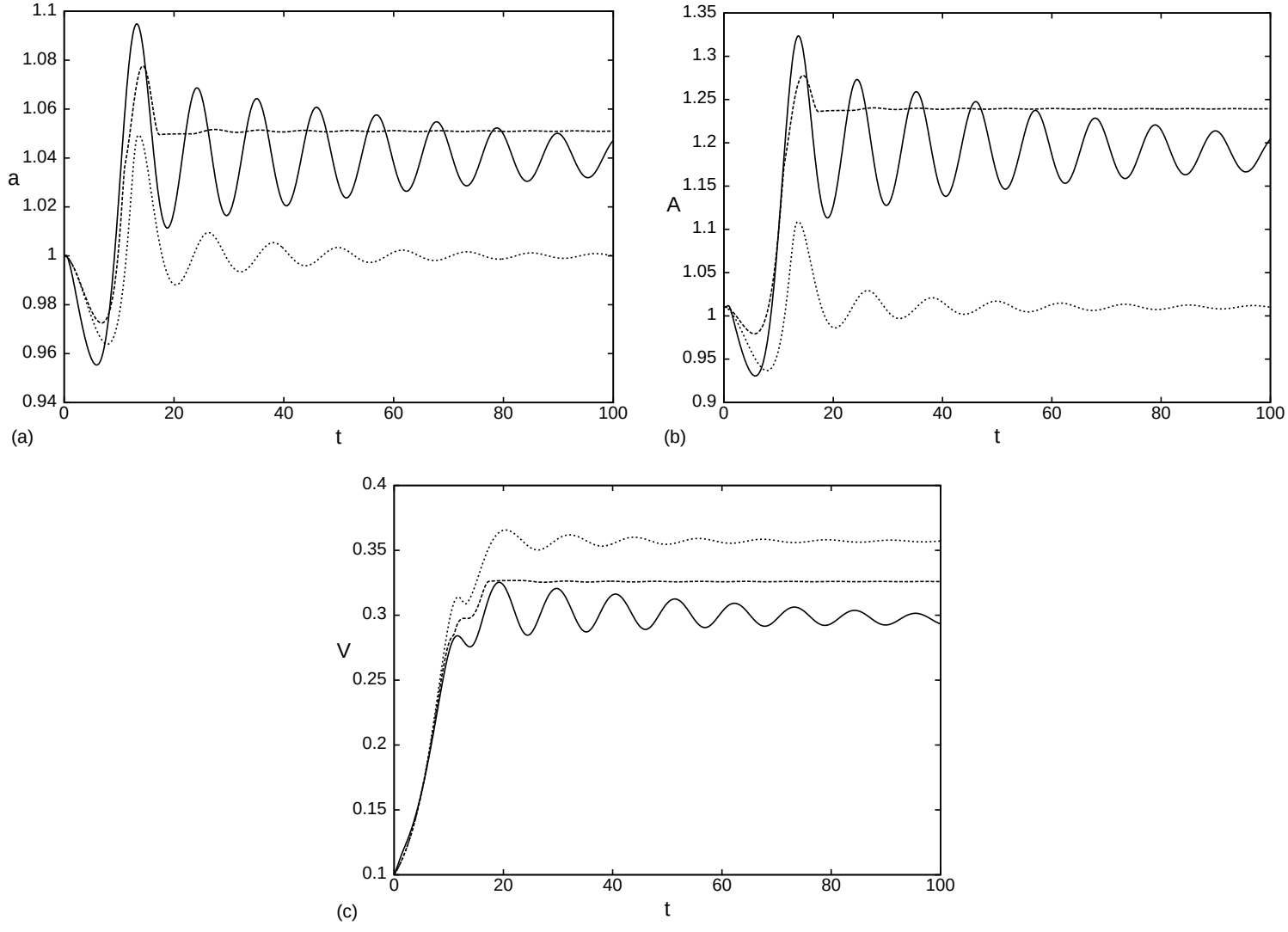

Fig. 3. Comparison between full numerical solution of Zakharov equations and solution of approximate equations for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.1$ for $x_1 = 1$, $x_2 = 2$, $f_1 = 0$ and $f_2 = 0.1$. (—) full numerical solution; (– – –) solution of approximate equations with loss to non-dispersive radiation; (- - -) solution of approximate equations with no loss to non-dispersive radiation. (a) Amplitude a of NLS soliton, (b) amplitude A of soliton in wave equation and (c) velocity V of the pulses.

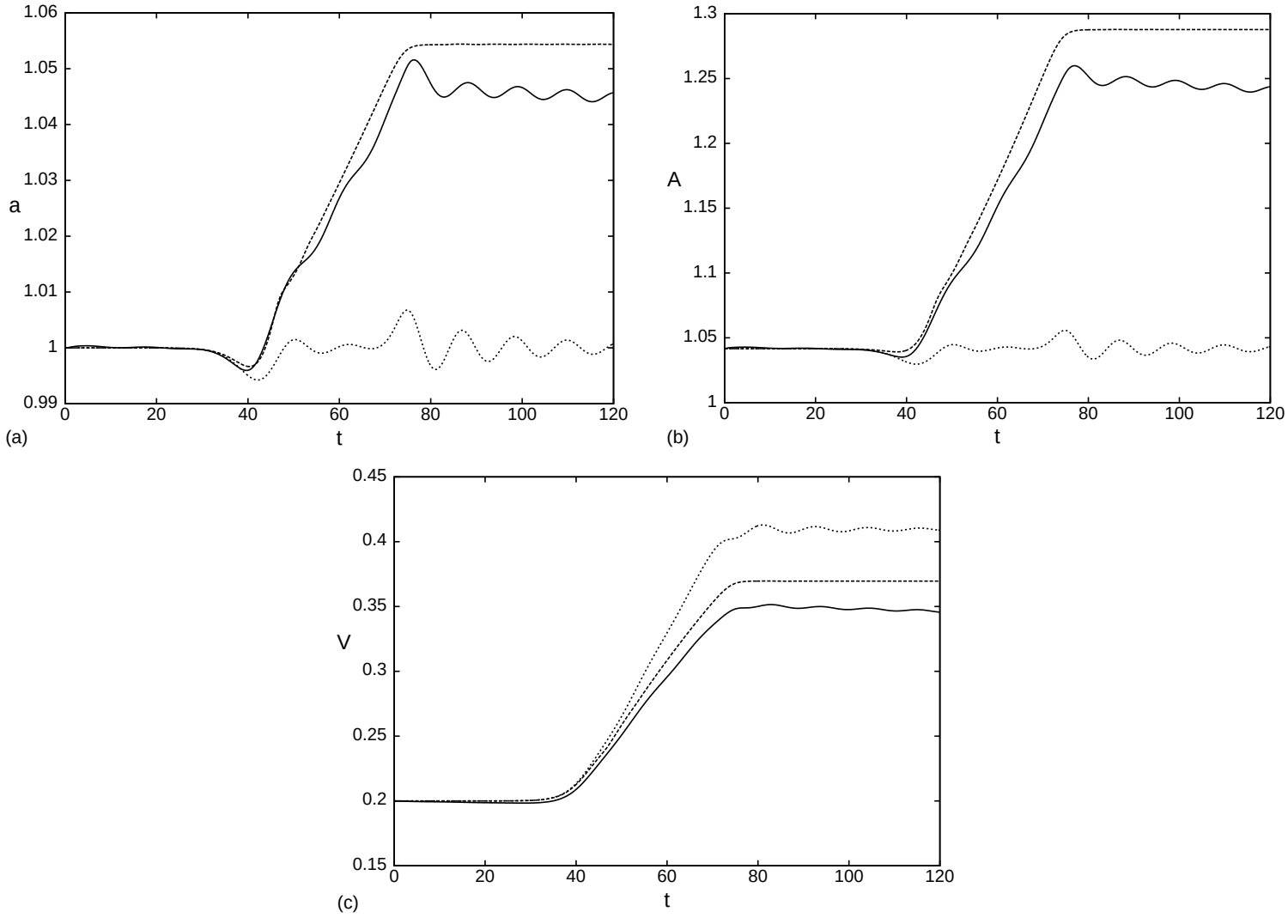

Fig. 4. Comparison between full numerical solution of Zakharov equations and solution of approximate equations for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.2$ for $x_1 = 8$, $x_2 = 18$, $f_1 = 0$ and $f_2 = 0.1$. (—) full numerical solution; (– – –) solution of approximate equations with loss to non-dispersive radiation; (- - -) solution of approximate equations with no loss to non-dispersive radiation. (a) Amplitude a of NLS soliton, (b) amplitude A of soliton in wave equation and (c) velocity V of the pulses.

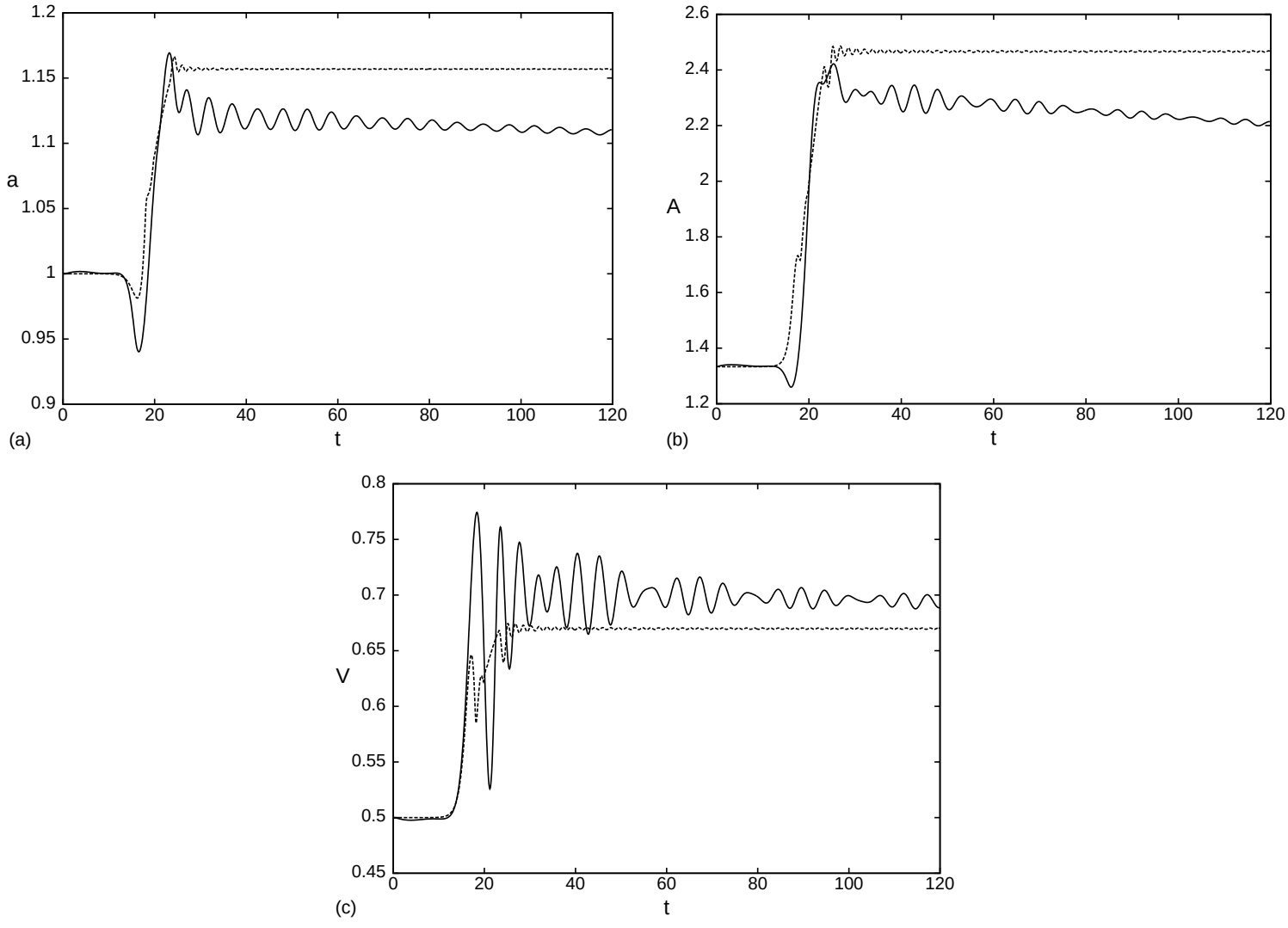

Fig. 5. Comparison between full numerical solution of Zakharov equations and solution of approximate equations for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.5$ for $x_1 = 8$, $x_2 = 13$, $f_1 = 0$ and $f_2 = 1.0$. (—) full numerical solution; (– – –) solution of approximate equations with loss to non-dispersive radiation. (a) Amplitude a of NLS soliton, (b) amplitude A of soliton in wave equation and (c) velocity V of the pulses.

the non-dispersive radiation loss is not as great in this case, but its inclusion leads to reasonable agreement with the full numerical solution. Again the damping of the velocity oscillations is too great in the approximate solution.

As the length of the inhomogeneous region becomes longer, the agreement between the approximate and full numerical solutions becomes better. This is because when the length of the inhomogeneous region is long compared with the soliton width, the soliton parameters are then slowly varying, which increases the validity of the approximate equations. This is particularly the case with the analysis of the effect of the hyperbolic radiation, which is based on V being slowly varying. Fig. 4 shows comparisons between the full numerical solution of the Zakharov equations and the solution of the approximate equations for such a long inhomogeneous region extending from $x_1 = 8$ to $x_2 = 18$. It can now be seen that there is excellent agreement between the full numerical and approximate solutions, as expected. In particular, the inclusion of the effect of the shed non-dispersive radiation is vital in order to obtain good agreement with the full numerical solution. Indeed, the non-dispersive radiation is much more important than the dispersive in driving the evolution of the Davydov soliton.

As the height of the inhomogeneity decreases and its slope increases, the velocity of the pulse approaches the sonic limit 1.0. Fig. 5 shows an example for which the inhomogeneity decreases by 1 over a distance $x_2 - x_1 = 5$. In this figure the approximate solution without non-dispersive radiation loss has not been shown as without non-dispersive radiation loss, the approximate velocity rapidly approaches 1 and the approximate equations become singular. Hence for large decreases in the inhomogeneity, the inclusion of the non-dispersive radiation loss is vital. It can be seen from Fig. 5(a) and (b) that there is excellent agreement between the full numerical and approximate solutions for the pulse amplitudes a and A, except that the period of the amplitude oscillations for the approximate solution is much shorter than the numerical period. The agreement for the velocity shown in Fig. 5(c) is good, with again the approximate oscillation period being much shorter than the numerical period. The numerical oscillations in A and V also show an anharmonic component. The initial conditions for $|E|$ and η and their full numerical solutions at $t = 120$ are shown in Fig. 6. It can be seen that the large change in the height of the inhomogeneity has caused a large precursor to develop ahead of the non-dispersive pulse. There is also a long, low precursor ahead of the

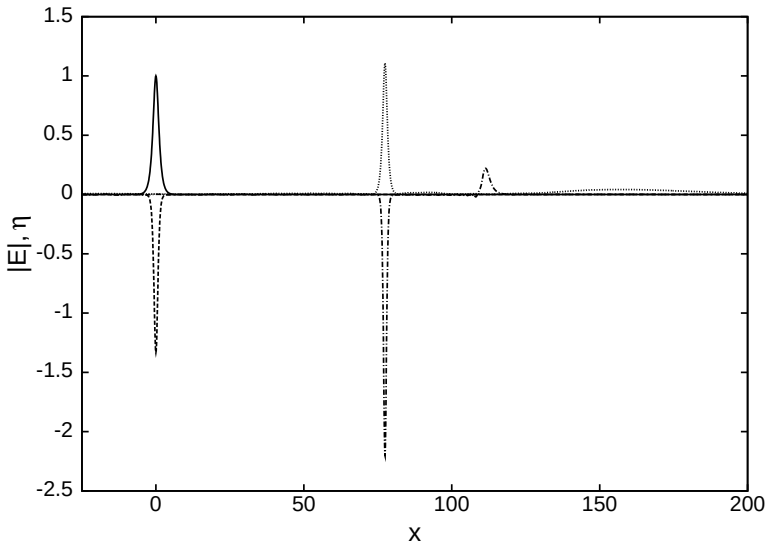

Fig. 6. Full numerical solution of the Zakharov equations (12) and (13) for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.5$ for $x_1 = 8$, $x_2 = 13$, $f_1 = 0$ and $f_2 = 1.0$. (—) initial condition for $|E|$; (– – –) initial condition for η; (- - -) solution for $|E|$ at $t = 120$; (– – –) solution for η at $t = 120$.

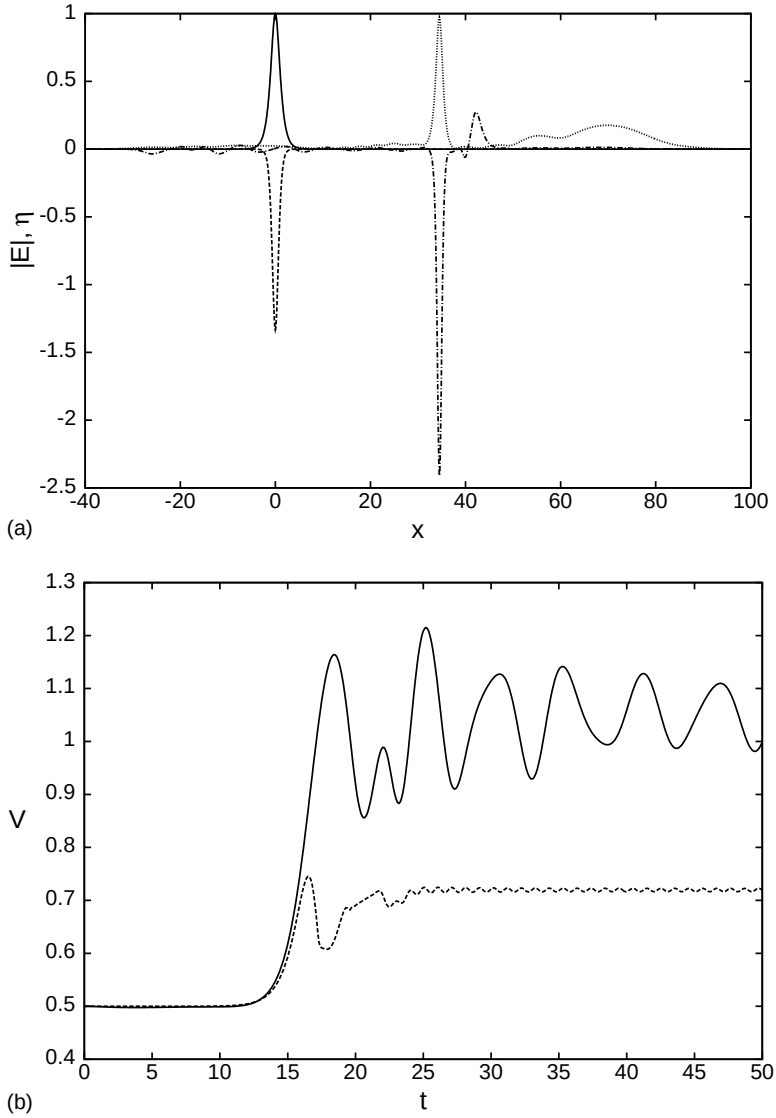

Fig. 7. Solution of the Zakharov equations (12) and (13) for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.5$ for $x_1 = 8$, $x_2 = 13$, $f_1 = 0$ and $f_2 = 2.0$. (a) Full numerical solution: (—) initial condition for $|E|$; (– – –) initial condition for η; (- - -) solution for $|E|$ at $t = 50$; (– – –) solution for η at $t = 50$. (b) Velocity of pulses: (—) full numerical solution; (- - -) solution of approximate equations with non-dispersive radiation loss.

NLS pulse. We finally note that these solutions for large inhomogeneity show that thermal fluctuations can have an important effect on the motion of a Davydov soliton and could even prevent its propagation.

Fig. 7 is for an even greater increase in the inhomogeneity, $f_1 = 0$ at $x_1 = 8$ and $f_2 = 2$ at $x_2 = 13$. Fig. 7(a) shows the initial conditions for $|E|$ and η and their full numerical solutions at $t = 50$. It can be seen that the NLS pulse has broken up, with a large precursor ahead of the main pulse. There is also a much smaller precursor ahead of the pulse in η. The reason for the break-up of the NLS pulse can be seen from Fig. 7(b). The full numerical solution shows that the velocity of the NLS pulse oscillates around $V = 1$. For $V > 1$, the NLS equation (12) becomes defocusing when coupled to a pulse solution $\eta(x - Vt)$ of the wave equation (13). Hence when $V > 1$, the NLS

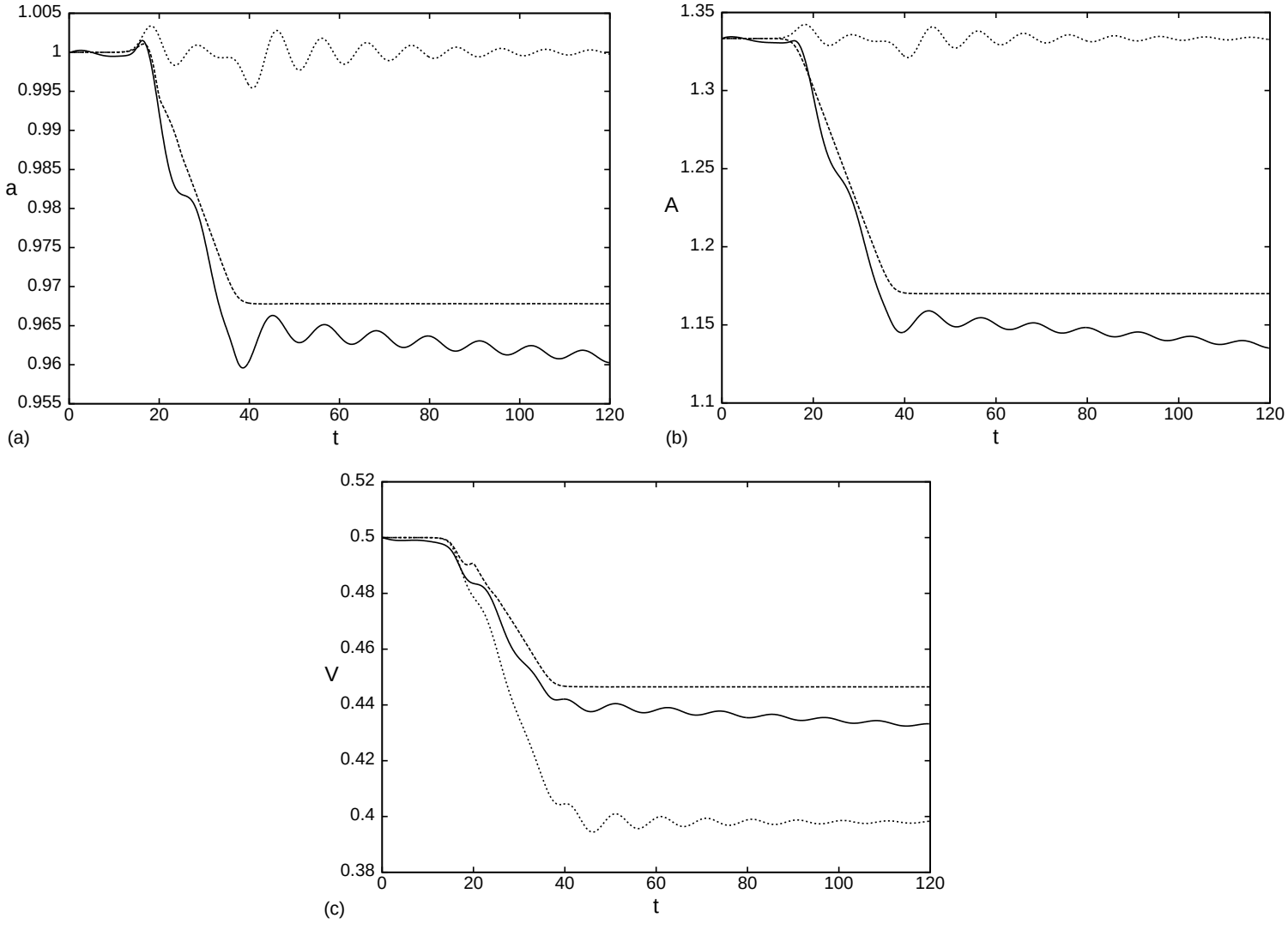

Fig. 8. Comparison between full numerical solution of Zakharov equations and solution of approximate equations for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.5$ for $x_1 = 8$, $x_2 = 18$, $f_1 = 0$ and $f_2 = -0.1$. (—) full numerical solution; (– – –) solution of approximate equations with loss to non-dispersive radiation; (- - -) solution of approximate equations with no loss to non-dispersive radiation. (a) Amplitude a of NLS soliton, (b) amplitude A of soliton in wave equation and (c) velocity V of the pulses.

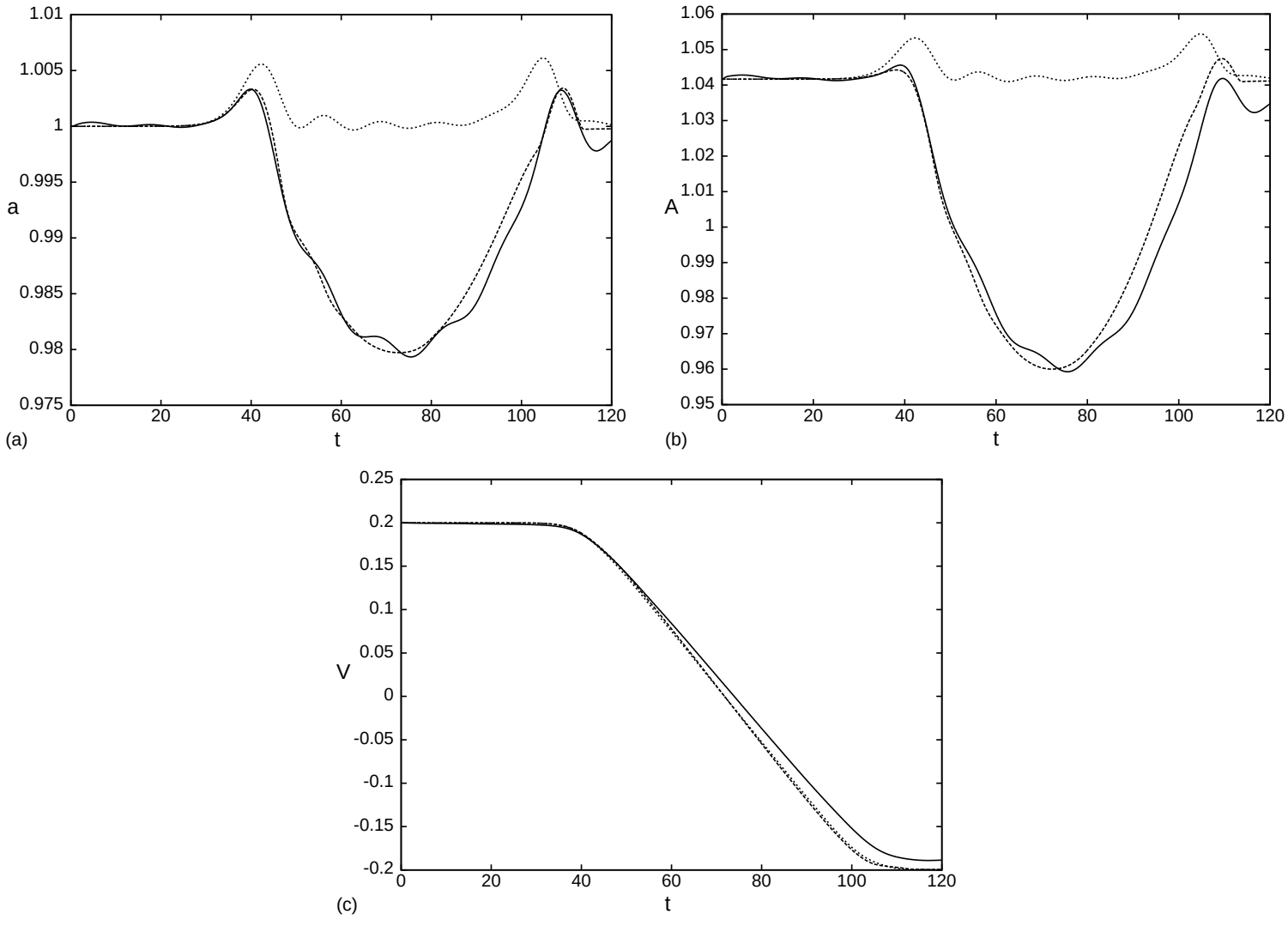

Fig. 9. Comparison between full numerical solution of Zakharov equations and solution of approximate equations for the initial conditions (22) with $a_0 = 1$ and $V_0 = 0.2$ for $x_1 = 8$, $x_2 = 18$, $f_1 = 0$ and $f_2 = -0.1$. (—) full numerical solution; (– – –) solution of approximate equations with loss to non-dispersive radiation; (- - -) solution of approximate equations with no loss to non-dispersive radiation. (a) Amplitude a of NLS soliton, (b) amplitude A of soliton in wave equation and (c) velocity V of the pulses.

pulse starts to break up. It can be seen from Fig. 7(b) that there is not good agreement between the full numerical and approximate solutions. However, good agreement is not expected as the approximate equations are not valid when the original pulses break up.

When there is decreasing inhomogeneity, so that $f_2 < f_1$, the Davydov soliton can evolve in two possible ways. For small initial velocities, the soliton will penetrate into the inhomogeneity and bounce back, while if the initial kinetic energy is larger than the height of the potential barrier, the soliton will go through the inhomogeneity.

Fig. 8 shows an example for which the initial kinetic energy is large enough so that the pulse can propagate through the decreasing inhomogeneity ($f_2 < f_1$). The inhomogeneous region itself is of length 10, $x_1 = 8$ and $x_2 = 18$, so that it is long compared with the soliton width. It can be seen from Fig. 8(a) and (b) that the agreement between the full numerical solution and the approximate solution with non-dispersive radiation loss for the pulse amplitudes a and A is reasonable, especially compared with the approximate solution without non-dispersive radiation loss. However, the agreement between the full numerical solution and the approximate solution with non-dispersive radiation loss for the pulse velocity V shown in Fig. 8(c) is excellent. Again the approximate solution without non-dispersive radiation loss is not in good agreement with the full numerical solution.

Fig. 9 shows comparisons between the full numerical solution of the Zakharov equations and the solution of the approximate equations for a long inhomogeneous region from $x_1 = 8$ to $x_2 = 18$ for which the inhomogeneity decreases and the Davydov soliton bounces back from it as it does not have enough initial kinetic energy. For this example of a soliton bouncing back from the inhomogeneity, the inclusion of loss to the shed non-dispersive radiation results in excellent agreement with the full numerical solution. This example shows the dominant effect of the non-dispersive radiation on the motion of the soliton. It can be seen from Fig. 9(c) showing the velocity evolution that non-dispersive radiation loss makes little difference to the pulse velocity.

6. Conclusions

Pulse propagation in a temperature gradient, governed by the non-integrable Zakharov equations has been studied and approximate equations derived for this evolution which include the coupling between the dispersive and non-dispersive waves. Since the Zakharov equations have a non-local Lagrangian, conservation laws were used to derive the approximate equations. However, while the Lagrangian was non-local, it did suggest the appropriate conservation equations to be used. Unlike previous studies of NLS-type equations, for which the radiation shed by an evolving pulse was purely dispersive [3,4,9,12], or the pulse equation is coupled to a diffusion equation [13], there was for the Zakharov equations radiative loss due to the non-dispersive (hyperbolic) nature of the wave equation. The main effect of this hyperbolic loss was on the soliton velocity. The hyperbolic waves shed by the pulse for the wave equation were found to carry a relatively large amount of mass and momentum. This was found to be the case even when the local acceleration of the pulse was small, but the accumulative effect of the inhomogeneity was large. It was found that temperature gradients do not destabilise the soliton, but can substantially alter its dynamics to the extent of preventing the propagation of the soliton and reversing its motion.

It was also shown that radiation processes which involve hyperbolic radiation have a very strong influence on the dynamics of the soliton.

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References

[1] X.-F. Pang, The lifetime of the soliton in the improved Davydov model at the biological temperature 300 K for protein molecules, Eur. Phys. J. B 19 (2001) 297–316.

[2] P.L. Christiansen, A.C. Scott (Eds.), Davydov's Soliton Revisited. Self Trapping of Vibrational Energy in Protein, NATO ASI Series, Series B: Physics, 243 (1990).

[3] W.L. Kath, N.F. Smyth, Soliton evolution and radiation loss for the nonlinear Schrödinger equation, Phys. Rev. E 51 (2) (1995) 1484–1492.

[4] J.J. Beech-Brandt, N.F. Smyth, Pulse evolution in nonlinear optical fibres with sliding-frequency filters, Phys. Rev. E 63 (2001) 056604-1–056604-11.

[5] A.S. Davydov, Solitons in Molecular Systems, 2nd ed. Kluwer Academic Publishers, Dordrecht, 1991.

[6] W.C. Kerr, P.S. Lomdahl, Quantum mechanical derivation of the Davydov equations for multi-quantum states, in: P.L. Christiansen, A.C. Scott (Eds.), Davydov's Soliton Revisited. Self Trapping of Vibrational Energy in Protein, NATO ASI Series, Series B: Physics 243 (1989).

[7] P.S. Lomdahl, W.C. Kerr, Davydov solitons at 300 K: the final search, in: P.L. Christiansen, A.C. Scott (Eds.), Davydov's Soliton Revisited, Self Trapping of Vibrational Energy in Protein, NATO ASI Series, Series B: Physics, 243 (1989).

[8] L. Cruzeiro-Hannson, P.L. Christiansen, A.C. Scott, Thermal stability of the Davydov soliton, in: P.L. Christiansen, A.C. Scott (Eds.), Davydov's Soliton Revisited, Self Trapping of Vibrational Energy in Protein, NATO ASI Series, Series B: Physics 243 (1989).

[9] N.F. Smyth, A.L. Worthy, Dispersive radiation and nonlinear twin-core fibres, J. Opt. Soc. Am. B 14 (10) (1997) 2610–2617.

[10] B. Fornberg, G.B. Whitham, A numerical and theoretical study of certain nonlinear wave phenomena, Phil. Trans. Roy. Soc. Lond. A 289 (1978) 373–403.

[11] M.J. Miksis, L. Ting, A numerical method for long time solutions of integro-differential systems in multi-phase flow, Comput. Fluids 16 (3) (1988) 327–340.

[12] N.F. Smyth, W.L. Kath, Radiative losses due to pulse interactions in birefringent nonlinear optical fibers, Phys. Rev. E 63 (2001) 036614-1–036614-9.

[13] C. García Reinbert, C. Garza Hume, A.A. Minzoni, N.F. Smyth, Active TM mode envelope soliton propagation in a nonlinear nematic waveguide, Physica D 167 (2002) 136–152.