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Anti-kink-like Propagation of Charge Carriers in Semiconductor Induced by Band-trap Impact Ionization

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Abstract: We investigate numerically a semiconductor nonlinear reaction-diffusion equation modeling the band-trap impact ionization phenomena. The factorization method is used to solve analytically this equation in order to derive some solutions for initial conditions for numerical simulation. As results, although the fact that electrons and holes shall recombine, we observe that they behave like anti-kink solitons propagating joined together without any destruction. Such behavior could stem from a local delicate balance between the generation and the recombination phenomena while the solitary waves are moving. Such carriers' behavior could lead to the introduction of many new semiconductor electronic devices that can be helpful in lossless signal transport, non-dissipative carriers transport in solar cells, and so on.

Keywords: Semiconductor; impact ionization; numerical simulation; anti-kink solitons

1 Introduction

Since it onset in sciences, the nonlinear science, also like quantum mechanics and relativity, has delivered a whole set of fundamentally new ideas and surprising results [1]. That science is found in all fields including either the scientific work or engineering fields. The domains such as fluid mechanics, plasma physics, optical fibers, biology, solid state physics, chemical kinematics, chemical physics, semiconductors carriers transport, and so on [2–5], are nonlinear sciences. Nonlinear science has begun to be a subject of a particular consideration for researchers since the discovery of the strange attractor and the solitary waves phenomena [6]. Nowadays, it is well known that waves play a pervasive role in nature. There are the mechanical waves, including seismic waves, sound waves in air, water waves. There are electromagnetic waves, and underlying all matter, quantum mechanical waves [7].

It is well known that many nonlinear phenomena and particularly waves, are described by nonlinear evolution equations (NLEEs) which help for their understanding. The investigation of the exact solutions of NLEEs and their numerical studies play an important role in the study of nonlinear physical phenomena. The exact solutions, if available, could be a helpful tool which will facilitate the verification of numerical solvers and aid in the stability analysis of solutions. The numerical investigation of NLEEs could be useful for the simulation and the understanding of the dynamics of phenomena that they descride.

There are many methods of investigation of exact solutions of NLEEs: the sine-cosine method [8–11], the tanh method [11], the Fan-expansion method [12], the (G'/G)-expansion method [13, 14], the modified mapping method, the extended mapping method [15], the Hirota Method [16] and the factorization method [17, 18], just to name a few. It is important to remark that among all those methods, the factorization method is more appropriate for handling nonlinear reaction-diffusion equations.

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Table 1: Material parameters corresponding to $\alpha - si$ near room temperature for the g-r process of band-trap impact ionization E_0 is the external applied field which can vary as a control parameter [20].

Parameters	value
X_1	$3 \times 10^{-5} exp(-\frac{2\times10^4}{E_0})\ Cm^3S^{-1}$
X_2	$3 \times 10^{-5} exp(-\frac{2.25\times10^4}{E_0})\ Cm^3S^{-1}$
B	$10^-10\ Cm^3S^{-1}$
N_D^*	$2 \times 10^{15}\ Cm^{-3}$
N_t	$3 \times 10^{15}\ Cm^{-3}$

In this paper, we deal with the following nonlinear reaction-diffusion equation [19]:

$$\frac{\partial n}{\partial t} - D_n \frac{\partial^2 n}{\partial x^2} = f_n(n,p), \tag{1a}$$

$$\frac{\partial p}{\partial t} - D_p \frac{\partial^2 p}{\partial x^2} = f_p(n,p), \tag{1b}$$

which models the electrons and holes transport in semiconductors under the effect of band-trap impact ionization. The parameters n, p, x and t stand for electrons and holes densities in the conduction and valence bands, the transverse coordinate and the time, respectively. The coefficients D_n and D_p are the electrons and holes diffusion constants; the functions f_n and f_p describe the generation-recombination (g-r) process of semiconductor band-trap impact ionization phenomenon; their simplest model [20] is given as follows:

$$f_n(n,p) = [X_1N_D^* - X_1n - (B - X_1)p]n, \tag{2a}$$

$$f_p(n,p) = [X_2P_D - X_2p - (B - X_2)n]p, \tag{2b}$$

with $P_D = N_t - N_D^*$. The parameters X_1 and X_2 are band-trap impact ionization coefficients, B is the band-band recombination coefficient. Also, the constants N_D^* and N_t are the effective donor density and the trap density, respectively.

For an n-type $\alpha - si$ which is operating near room temperature, we have $D_n = 35cm^2s^{-1}$, $D_p = 12.4cm^2s^{-1}$ and all the above coefficients are explicitly given by Table 1.

Semiconductors are one of the most used materials that support our nowadays technology. Many electronic devices designed for various purposes are made of semiconductor materials. The working principles of those devices are generally based on the nonlinear behaviors of charge carriers in semiconductors. That behaviors most often stem from the g-r phenomena which is a self organizing process supported by nonequilibrium phase transitions in semiconductors. In previous works, we have investigated exact solitary solutions of semiconductors one level impact ionization equation [21] and that solutions were found to be helpful for non-dissipative conduction in semiconductors. Optical solitary waves have been investigated in semiconductors and find their applications in many domains such as optical fibers. We believe that, many other applications could be found by means of the investigation of new charge carriers solitary behaviors.

In this work we aim to study by means of numerical simulation the propagation of anti-kink soliton in $\alpha - si$ induced by band-trap impact ionization phenomena. To reach such a purpose, we derive by means of the factorization method, the exact solutions of the Eq. (1) and used them for numerical studies.

Therefore, we outline this paper as follows, the section 2 will deal with the brief presentation of the factorization method. The section 3 will treat the application of this method to the Eq. (1). In section 4, the numerical studies will be presented. The paper ends with the section 5 which is devoted to important remarks and conclusion.

2 Brief Presentation of the factorization Method

The factorization Method [18] is based on the factorization technic of systems of differential equations. Let us consider the following set of differential equations

$$u^{''} + g_1(u,v)u^{'} + f_1(u,v) = 0, \tag{3a}$$

$$v^{''} + g_2(u,v)v^{'} + f_2(u,v) = 0, \tag{3b}$$

where the prime symbol ($'$) represents $D = \frac{\partial}{\partial z}$, and the functions $g_i(u,v), f_i(u,v), (i = 1, 2)$ are polynomials in u and v; it can be rewritten as follows:

$$(D^2 + g_1(u,v)D + \frac{f_1(u,v)}{u})u = 0, \tag{4a}$$

$$(D^2 + g_2(u,v)D + \frac{f_2(u,v)}{v})v = 0. \tag{4b}$$

When $f_1(u,v) = uh_1(u,v)$ and $f_2(u,v) = vh_2(u,v)$, equation (4) can be factorized as:

$$(D - \psi_{12}(u,v))(D - \psi_{11}(u,v))u = 0, \tag{5a}$$

$$(D - \psi_{21}(u,v))(D - \psi_{22}(u,v))v = 0. \tag{5b}$$

The equation (5) can be developed and leads to,

$$u^{''} - (\psi_{12} + \psi_{11} + \frac{\partial \psi_{11}}{\partial u}u)u^{'} + u\psi_{11}\psi_{12} = 0, \tag{6a}$$

$$v^{''} - (\psi_{21} + \psi_{22} + \frac{\partial \psi_{22}}{\partial v}v)v^{'} + v\psi_{22}\psi_{21} = 0. \tag{6b}$$

By identifying each member of equation (3) to those of (6) we obtain:

$$g_1(u,v) = -(\psi_{12} + \psi_{11} + \tfrac{\partial \psi_{11}}{\partial u}u), \tag{7a}$$

$$g_2(u,v) = -(\psi_{21} + \psi_{22} + \tfrac{\partial \psi_{22}}{\partial v}v), \tag{7b}$$

$$f_1(u,v) = u\psi_{12}\psi_{11}, \tag{7c}$$

$$f_2(u,v) = v\psi_{21}\psi_{22}. \tag{7d}$$

The functions g_1 and g_2 must have the same order as $\psi_{12}, \psi_{11}, \psi_{21}$, and ψ_{22} for f_1 and f_2 polynomials. The relation (7) will be useful in the determination of constant parameters. The development of Eq. (5) yields four systems of first order differential equations

$$u^{'} - \psi_{11}(u,v)u = 0, \quad v^{'} - \psi_{22}(u,v)v = 0, \tag{8a}$$

$$u^{'} - \psi_{12}(u,v)u = 0, \quad v^{'} - \psi_{22}(u,v)v = 0, \tag{8b}$$

$$u^{'} - \psi_{12}(u,v)u = 0, \quad v^{'} - \psi_{21}(u,v)v = 0, \tag{8c}$$

$$u^{'} - \psi_{11}(u,v)u = 0, \quad v^{'} - \psi_{21}(u,v)v = 0. \tag{8d}$$

A particular solution of equation (3) can be obtained through an appropriate choice of ψ_{11} and ψ_{22}.

3 Discussion of the factorization method to a semiconductor nonlinear reaction-diffusion equation describing band-trap impact ionization

For traveling waves, we set, $z = x - ct$ with c the propagation speed, then Eq. (1) can be turned to

$$\frac{\partial^2 n}{\partial z^2} + \frac{c}{D_n}\frac{\partial n}{\partial z} + \frac{f_n}{D_n} = 0, \tag{9a}$$

$$\frac{\partial^2 p}{\partial z^2} + \frac{c}{D_p}\frac{\partial p}{\partial z} + \frac{f_p}{D_p} = 0. \tag{9b}$$

Furthermore, we set

$$g_1(n,p) = \tfrac{c}{D_n}, \tag{10a}$$

$$g_2(n,p) = \tfrac{c}{D_p}, \tag{10b}$$

$$f_1(n,p) = n\psi_{12}\psi_{11}, \tag{10c}$$

$$f_2(n,p) = p\psi_{21}\psi_{22}. \tag{10d}$$

For $n \neq 0$ and $p \neq 0$ we factorize eq(9) as follows:

$$(D - \psi_{12}(n,p))(D - \psi_{11}(n,p))n = 0, \quad (11a)$$
$$(D - \psi_{21}(n,p))(D - \psi_{22}(n,p))p = 0. \quad (11b)$$

By choosing ψ_{ij} such as,

$$\psi_{11}(n,p) = k_1 X_1(N_D^* - n), \quad \psi_{12}(n,p) = \frac{1}{k_1 D_n}(1 - \frac{(B-X_1)P}{X_1(N_D^*-n)}), \quad (12a)$$
$$\psi_{22}(n,p) = k_2 X_2(P_D - p), \quad \psi_{21}(n,p) = \frac{1}{k_2 D_p}(1 - \frac{(B-X_2)n}{X_2(P_D-p)}), \quad (12b)$$

where we have suppose once more $n \neq N_D^*$ and $p \neq P_D$. The constants k_1 and k_2 are given by the first condition of the equalities (7a) and (7b):

$$k_1 = \frac{-\frac{c}{D_n} \pm \sqrt{\Delta_1}}{2X_1 N_D^*}, \quad \Delta_1 = (\frac{c}{D_n})^2 - 4\frac{X_1 N_D^*}{D_n}, \quad (13a)$$
$$k_2 = \frac{-\frac{c}{D_p} \pm \sqrt{\Delta_2}}{2X_2 P_D}, \quad \Delta_2 = (\frac{c}{D_p})^2 - 4\frac{X_2 P_D}{D_p}. \quad (13b)$$

According to [18], the compatible first order system of differential equations is

$$n^{'} - k_1 X_1(N_D^* - n)n = 0, \quad (14a)$$
$$p^{'} - k_2 X_2(P_D - p)p = 0. \quad (14b)$$

The eq(14a) and eq(14b) are Bernoulli equations, then their solutions are as follows:

$$n_+(z) = \frac{N_D^*}{2}[1 + \tanh((\frac{-c}{4D_n} \pm \frac{\sqrt{\Delta_1}}{4})(z - z_0))], \quad (15a)$$
$$n_-(z) = \frac{N_D^*}{2}[1 + \coth((\frac{-c}{4D_n} \pm \frac{\sqrt{\Delta_1}}{4})(z - z_0))], \quad (15b)$$
$$p_+(z) = \frac{P_D}{2}[1 + \tanh((\frac{-c}{4D_p} \pm \frac{\sqrt{\Delta_2}}{4})(z - z_0))], \quad (15c)$$
$$p_-(z) = \frac{P_D}{2}[1 + \coth((\frac{-c}{4D_p} \pm \frac{\sqrt{\Delta_2}}{4})(z - z_0))], \quad (15d)$$

with z_0 the phase boundary.

4 Numerical simulation of anti-kink propagation in α-si

We use the Matlab partial differential equations solver and solutions (15a) and (15c),

$$n_+(z) = \frac{N_D^*}{2}[1 + \tanh((\frac{-c}{4D_n} \pm \frac{\sqrt{\Delta_1}}{4})(x))], \quad (16a)$$
$$p_+(z) = \frac{P_D}{2}[1 + \tanh((\frac{-c}{4D_p} \pm \frac{\sqrt{\Delta_2}}{4})(x))], \quad (16b)$$

as initial conditions to simulate the anti-kink propagation in Eq. (1a). The phase boundary z_0 for simplicity is set to 0. we obtain the Fig. 1 for the electrons propagating like an anti-kink soliton at the phase speed of c=500 and $E_0 = 1500V/cm$.

Holes also propagate like an anti-kink soliton in Fig. 2.

It is important to remark that the " holistic " anti-kink and the " electronic " one are joined, ie they are moving together from one point to another. The Fig. 3 presents the two solitons moving together.

To clearly observe this phenomena we change the direction of propagation of the " holistic " anti-kink by choosing the following initial condition,

$$n_+(z) = \frac{N_D^*}{2}[1 + \tanh((\frac{-c}{4D_n} \pm \frac{\sqrt{\Delta_1}}{4})(x))], \quad (17a)$$
$$p_+(z) = \frac{P_D}{2}[1 + \tanh((\frac{-c}{4D_p} \pm \frac{\sqrt{\Delta_2}}{4})(-x))]. \quad (17b)$$

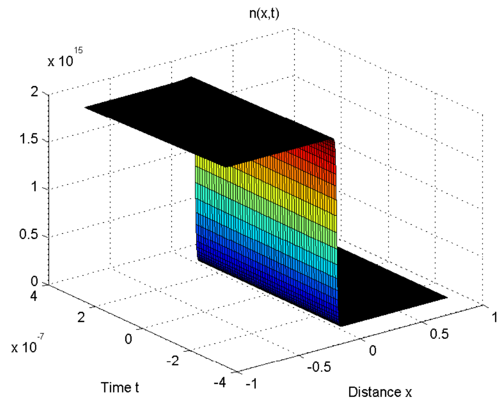

Figure 1: “ Electronic ” anti-kink soliton propagating at the phase speed of c=500 and for $E_0 = 1500V/cm$.

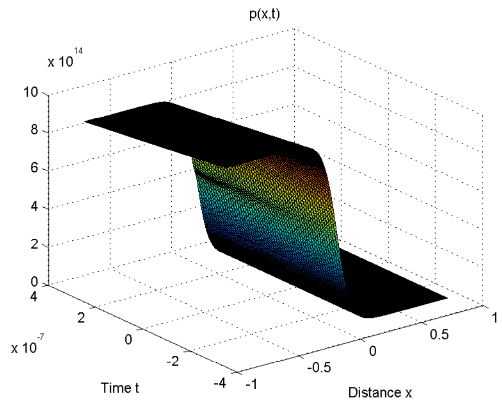

Figure 2: “ Holistic ” anti-kink soliton propagating at the phase speed of c=500 and for $E_0 = 1500V/cm$.

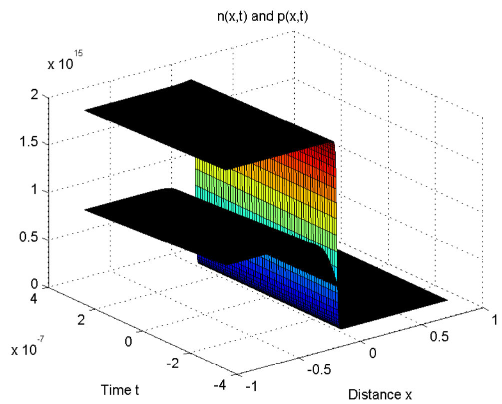

Figure 3: “ Electronic ” and “ holistic ” anti-kink soliton propagating together in the same direction.

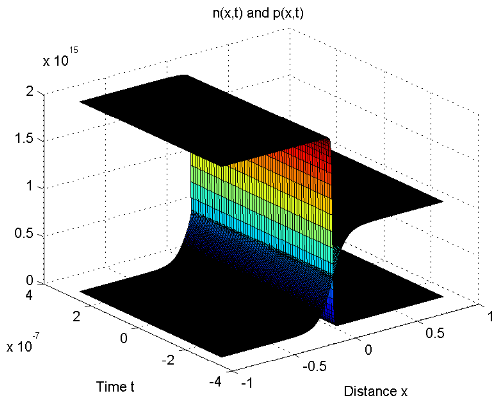

Figure 4: " Electronic " and " holistic " anti-kink soliton propagating together. The direction of " holistic " one is inverted.

This yields the graph of the Fig. 4.

Normally when an electron encounters a hole, it has to recombine it. This can lead us to think that some electrons and holes in the solitary waves may recombine and then lead to the destruction of the waves. But we observe here that there is not any destruction. From this, we may assert that electrons and holes do not recombine while solitary waves are moving and then conclude that the solitary nature of the carriers motion, prevail on the recombination phenomena. But this is not real.

We believe that in order to observe such simultaneous " holistic " and " electronic " anti-kink propagation, a delicate balance between the generation and the recombination phenomena is established. This is although the fact that the entire semiconductor is not at equilibrium, that is in thermodynamics equilibrium or in a stationary state, there is a local equilibrium between the generation and the recombination phenomena where the solitary waves pass. While the anti-kinks are moving, the same number of electrons and holes which are captured from it by the traps is the same number that are set free from traps to solitary waves. Also the amount of carriers which are lost from the anti-kinks by recombination are exactly replace by the generation phenomena.

5 Conclusion

In this work, we focused on the numerical simultaneous " holistic " and " electronic " anti-kink propagation in a $\alpha - si$. The analytical treatment of the Eq. (1) leads to the solutions (15). These solutions can further be divided in two classes by considering that Δ_1 and Δ_2 can also be negative. For $\Delta_1 < 0$ and $\Delta_2 < 0$ the $\tanh$ and the $\coth$ functions can be turned to rational functions of $\cosh$ and $\sinh$ and then lead to the observation of other kind of solitons.

Here, we did not deal with the $\coth$ solutions because they are very delicate to manipulate and do not lead to interesting results. They introduce some singularities in the Eq. (1) and lead the integrator to fail. This singularity is related to the first order phase transitions occurring in the semiconductor since the Eq. (1) describe the switching phenomena semiconductors.

At the end of this study, we realize that " holistic " and " electronic " anti-kink propagate simultaneously in the same space because of delicate balance between the generation and the recombination phenomena. This carriers behavior could lead to the introduction of many new semiconductor electronic devices that can be helpful in lossless signal transport, non-dissipative carriers transport in solar cells.

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