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J. Phys. A: Math. Theor. 42 (2009) 485211 (17pp)

doi:10.1088/1751-8113/42/48/485211

New solutions for the quantum drift-diffusion model of semiconductors

J Ramírez¹ and R Tracinà²

¹ Departamento de Matemáticas, Universidad de Cádiz, Puerto Real, Cádiz, Spain

² Dipartimento di Matematica e Informatica, Viale A. Doria 6, 95125 Catania, Italy

E-mail: pepe.ramirez@uca.es and tracina@dmi.unict.it

Received 22 May 2009, in final form 21 September 2009 Published 17 November 2009 Online at stacks.iop.org/JPhysA/42/485211

Abstract

In this paper new symmetry reductions and exact solutions are found for the one-dimensional quantum drift–diffusion model for semiconductors based on the Bohm potential. The symmetry reductions are derived by using the nonclassical method developed by Bluman and Cole. Further reductions are obtained by means of other types of symmetry reductions or by *ansatz*-based reductions. In particular, several types of exact solutions are derived: kinks, *k*hump compactons and elliptic traveling waves. The new solutions can display several types of coherent structures.

PACS numbers: 02.30.Jr, 02.20.Sv

1. Introduction

Classical drift–diffusion and energy transport models describe the transport of charged species in strong interaction with a surrounding medium. Such situations occur in semiconductors (where electrons and holes are interacting with the crystal impurities) or in cold plasma or gas discharges (where the electrons and ions are interacting with the surrounding neutral molecules). Nowadays, quantum effects play an important role in semiconductor devices. The ongoing progress of industrial semiconductor device technologies permits us to fabricate devices which inherently employ quantum phenomena in their operation, e.g. resonant tunneling diodes, quantum well laser, etc. Some device architectures are based in ultra thin body silicon-on-insulator FETs where a structural confinement of the carrier gas is taking place in one or two dimensions.

A proper description of the device electrostatic and current transport requires quantum effects to be accounted for. The widely used drift–diffusion equation introduced by van Roosbroeck [22] in 1950 is not capable of taking these quantum effects into account properly. Several finer levels of modeling have been used: Schrödinger or collisional Wigner equation, hybrid models. The last ones use a quantum model in regions where the quantum effects

1751-8113/09/485211+17\$30.00 © 2009 IOP Publishing Ltd Printed in the UK

take place and couple this model by proper interface condition (e.g. continuity of the electron and current densities) to a classical drift-diffusion or hydrodynamic model in the reminder. This approach is referred to as *quantum drift-diffusion*. A simplified version of it, which replaces the Schrödinger equation by a nonlinear equation in the electron-charge distribution, is sometimes called density-gradient models. Continuum models for the description of charge carrier transport in semiconductors are of a major interest for applied mathematicians and engineers, on account of their applications to the design of electron devices. The driftdiffusion models are also widely used in engineering applications [6, 11, 21]. These models are obtained by the balance equation for electron density and/or hole density coupled to the Poisson equation for the electric potential. The classical drift-diffusion models have been thoroughly investigated from an analytical point of view [7, 8, 11, 15] and several suitable efficient numerical methods have been developed [4].

Due to the complexity of the model, the quantum drift–diffusion equations are usually solved numerically. Another approach to solve them analytically has been carried out by perturbation methods [20]. Recently, in [17], approximate solutions to the quantum drift–diffusion model for semiconductors have been found with the aid of the symmetry group analysis performed in [16].

Symmetry group techniques, in general, provide a method for obtaining exact analytical solutions of partial differential equations (PDEs) and can be used to reduce the number of dependent and/or independent variables. From a known solution of a differential equation, and by applying symmetry transformations, several classes of new solutions can be obtained; in fact, quite often, interesting solutions can be obtained from trivial ones.

The classical method for finding symmetry reductions of PDEs is the Lie group method of infinitesimal transformations. In this case the associated determining equations are an overdeterminated linear system of equations [3, 12, 13]. Motivated by the fact that there are symmetry reductions of PDEs that cannot be obtained by using the classical Lie group method, several generalizations of this method have been developed. Bluman and Cole [2] introduced the nonclassical method to study the heat equation. One can show that all the classical symmetry are also nonclassical ones because they satisfy the invariance surface conditions. For the nonclassical method, the determining system is usually highly nonlinear, so a complete analysis of the nonclassical symmetries can rarely be done. The method of nonclassical reduction has been used to find new exact solutions of many nonlinear partial differential equations of physical or mathematical relevance (e.g. [9, 5, 14]).

If we are able to find a solution of the determining equations then we obtain the explicit form of a vector field *Y*, which is named as a *nonclassical symmetry operator*. In general, the corresponding local point transformations do not leave the system invariant; i.e. they will not transform solutions amongst each other, but transform solutions which satisfy invariance surface conditions into solutions verifying the same conditions.

For several classes of PDE, the search of soliton-like solutions has raised a great interest during the last two decades. Solitons are analytical solutions that are exponentially localized in the space, but, in general, they are not null out of any bounded set. By weakening the regularity conditions and by strengthening the conditions of localization, the compactons were introduced [10, 19]. The functions in this class are null out of some bounded spatial set but may be not analytical at some points.

For nonlinear PDE whose coefficients vanish at some points, as is our drift-diffusion model, the existence and relevance of non-analytical solutions have been considered by several authors. However, some of these authors do not always use the same definitions to deal with compactons. The main differences appear with the behavior of the possible solutions at the singularities of the equation. In this paper we understand that a compacton is a function that

has enough continuous derivatives in order for this function to satisfy the PDE in *all* points [18]. Of course, at the singularities the hypothesis of the Cauchy–Kovalevsky theorem is not satisfied.

This paper is organized as follows. At the beginning, in section 2, we describe the quantum drift-diffusion model. In section 3, by applying the infinitesimal method, we obtain some nonclassical symmetries for the quantum drift-diffusion model of semiconductors in the one-dimensional case, and, after the corresponding symmetry reductions, we obtain several classes of particular solutions. In section 4 we study some qualitative aspects of the classes of solutions that we have found: kinks, kink-antiking structures, periodic nets of dromions-antidromions, compactons, etc.

2. The quantum drift-diffusion model

When the dimensions of submicron semiconductor devices are shrunk, the quantum effects are no longer negligible and a way to include them is based on the Bohm potential. The resulting quantum drift–diffusion model [8] is given in the unipolar case by the system

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J} = 0, \tag{1}$$

$$\lambda^2 \Delta \Phi = n - c(\mathbf{x}),\tag{2}$$

where *n* is the electron density, **J** is the electron momentum density, λ^2 is the dielectric constant divided by the elementary charge *e*, Φ is the electric potential and $c(\mathbf{x})$ is the doping concentration as a function of the position **x**. As usual, ∇ denotes the divergence operator and Δ is the Laplacian with respect to spatial variables.

The constitutive relation for the momentum density \mathbf{J} is expressed as the sum of a diffusion, a drift and a quantum term

$$\mathbf{J} = -K\,\nabla(n^{\alpha}) + \mu\,n\,(\nabla\Phi + \nabla Q),\tag{3}$$

where *K* is the diffusion coefficient, μ is the mobility and *Q* is the Bohm quantum correction. This correction *Q* can be expressed as

$$Q = H_0 \frac{\Delta \sqrt{n}}{\sqrt{n}},\tag{4}$$

where $H_0 = \frac{\hbar}{2m^* e}$, \hbar being the reduced Planck constant and m^* the effective electron mass. The constant α must satisfy the condition $\alpha \ge 1$. The limit case $\alpha = 1$ is the quantum analogous of the isothermal flow, which is the basic assumption in the classical drift–diffusion models.

As usual, we assume that K and μ are related by the Einstein relation

$$K = U_0 \mu, \tag{5}$$

where $U_0 = \frac{k_B T_L}{e}$ is the constant thermal potential, k_B being the Boltzmann constant and T_L the lattice temperature attained at equilibrium.

The mobility μ is considered to be a function of the modulus |E| of the electric field $E = -\nabla \Phi$; i.e.

$$\mu = \mu(|E|). \tag{6}$$

From the mathematical point of view, this kind of model can be considered as a fourthorder parabolic equation coupled by an elliptic equation. In the one-dimensional case the Poisson equation can be rewritten as follows. Since $n \ge 0$, we will use a new variable w so that $w^2 = n$. Then, the system in the dependent variables w and E becomes

$$S_{1} \equiv \frac{\partial w^{2}}{\partial t} + \frac{\partial}{\partial x} \left(-\mu U_{0} \frac{\partial w^{2\alpha}}{\partial x} - \mu w^{2} E + \mu H_{0} \left(w \frac{\partial^{3} w}{\partial x^{3}} - \frac{\partial^{2} w}{\partial x^{2}} \frac{\partial w}{\partial x} \right) \right) = 0, \tag{7}$$

$$S_2 \equiv \lambda^2 \frac{\partial E}{\partial x} + w^2 - c(x) = 0.$$
(8)

From now on, we consider μ depending on *E* and, to consider solutions with physical relevance, when μ is nonconstant we must require that *E* is either positive or negative.

3. Nonclassical symmetries and exact solutions

In order to obtain new solutions of system (7)–(8), we apply the nonclassical method of reduction. We consider a one-parameter Lie group of infinitesimal transformations of the form

$$Y = \xi(t, x, w, E) \frac{\partial}{\partial x} + \tau(t, x, w, E) \frac{\partial}{\partial t} + \eta_1(t, x, w, E) \frac{\partial}{\partial w} + \eta_2(t, x, w, E) \frac{\partial}{\partial E}.$$
 (9)

We require that (9) leaves invariant equations (7) and (8) and the invariance surface conditions

$$\xi w_x + \tau w_t - \eta_1 = 0, \qquad \xi E_x + \tau E_t - \eta_2 = 0, \tag{10}$$

where the subscripts t and x represent the partial derivatives with respect to t and x, respectively.

This leads to a complicated nonlinear system of determining equations for the functions $\xi(t, x, w, E), \tau(t, x, w, E), \eta_1(t, x, w, E)$ and $\eta_2(t, x, w, E)$.

In order to analyze the set of determining equations, we will consider two cases: $\tau \neq 0$ and $\tau = 0$.

3.1. Case 1. $\tau = 0$

When $\tau = 0$, without loss of generality, we can assume that $\xi(t, x, w, E) = 1$. In this case the invariant surface conditions (10) reduce to

$$w_x = \eta_1,\tag{11}$$

$$E_x = \eta_2. \tag{12}$$

By (12), equation (8) becomes a non differential equation:

$$\eta_2 = \frac{c(x) - w^2}{\lambda^2},\tag{13}$$

and system (7)–(8) is reduced to a single equation. In this case, the symmetry operator adopts the following form:

$$Y = \frac{\partial}{\partial x} + \eta_1(t, x, w, E) \frac{\partial}{\partial w} + \frac{c(x) - w^2}{\lambda^2} \frac{\partial}{\partial E},$$
(14)

where the coordinate η_1 must satisfy a complicated nonlinear partial differential equation. We are able to obtain only some particular solutions and the corresponding symmetry reductions.

Symmetry reduction 1.1. For $\alpha \neq 1$, c(x) arbitrary and $\mu(E) = \frac{\mu_0}{E}$, with μ_0 a constitutive constant, we have

$$\eta_1 = \pm \sqrt{\frac{U_0}{(\alpha - 1)H_0}} w^{\alpha}.$$
(15)

In this case, in order to obtain the similarity variables associated with generator (14), we set $\beta = \sqrt{\frac{(\alpha - 1)U_0}{H_0}}$ and we distinguish two subcases.

(1) If $\alpha = 3$, the new variables are y = t, $w = [-\beta x + u(y)]^{-1/2}$, $E = v(y) + \frac{A(x)}{\lambda^2} + \frac{\ln(-\beta x + u)}{\lambda^2 \beta}.$ (16)

(2) If $\alpha \neq 3$, the new variables are y = t, $w = [-\beta x + u(y)]^{1/(1-\alpha)}$,

$$E = v(y) + \frac{A(x)}{\lambda^2} + \frac{(1-\alpha) [-\beta x + u]^{\frac{3-\alpha}{1-\alpha}}}{(3-\alpha)\lambda^2\beta}.$$
 (17)

In both cases v(y) is an arbitrary function, the functions A(x), u(y) must satisfy

$$A'(x) = c(x); \qquad u' = -\mu_0 \sqrt{\frac{(\alpha - 1)U_0}{H_0}}.$$
(18)

By solving (18) we get $u = -\mu_0 \sqrt{\frac{(\alpha - 1)U_0}{H_0}} y + a_1$, where a_1 is an arbitrary constant.

The corresponding solutions of system (7)–(8) are given by $w = [-\beta(x + \mu_0 t) + a_1]^{\frac{1}{1-\alpha}}$ and

(1) if $\alpha = 3$,

$$E = v(t) + \frac{A(x)}{\lambda^2} + \frac{\ln(-\beta(x+\mu_0 t) + a_1)}{\lambda^2 \beta};$$
(19)

(2) if $\alpha \neq 3$,

$$E = v(t) + \frac{A(x)}{\lambda^2} + \frac{1 - \alpha}{(3 - \alpha)\lambda^2\beta} [-\beta(x + \mu_0 t) + a_1]^{\frac{3 - \alpha}{1 - \alpha}};$$
 (20)

where $\beta = \sqrt{\frac{(\alpha-1)U_0}{H_0}}$.

Symmetry reduction 1.2. For $\alpha = 2$, $c(x) = c_0 e^{\mp \frac{x}{\lambda \sqrt{2U_0}}}$ and $\mu(E) = \mu_0$, with c_0 and μ_0 constitutive constants, we get

$$\eta_1 = \pm \frac{w}{2\lambda\sqrt{2U_0}}.\tag{21}$$

In this case the new variables are

$$y = t,$$
 $w = u(y) e^{\frac{\pm x}{2\lambda\sqrt{2U_0}}},$ $E = v(y) \mp \frac{\sqrt{2U_0}}{\lambda} \left(e^{\pm \frac{x}{\lambda\sqrt{2U_0}}} u(y)^2 + c_0 e^{\mp \frac{x}{\lambda\sqrt{2U_0}}} \right),$ (22)

where u, v must satisfy the equation

$$\mu_0 \, u \, v \mp 2\lambda \sqrt{2U_0} u' = 0. \tag{23}$$

When u(t) is arbitrary, the corresponding solution of system (7)–(8) is

$$w = u(t) e^{\frac{2\lambda}{2\lambda}\sqrt{2U_0}},$$

$$E = \pm \frac{2\lambda\sqrt{2U_0} u'(t)}{\mu_0 u(t)} \mp \frac{\sqrt{2U_0}}{\lambda} e^{\pm \frac{x}{\lambda\sqrt{2U_0}}} (u(t)^2 + c_0 e^{\mp \frac{2x}{\lambda\sqrt{2U_0}}}).$$
(24)

Symmetry reduction 1.3. For $\alpha = 3/2$, c(x) arbitrary and $\mu(E) = \frac{\mu_0}{3\mu_1 U_0 + E}$, with μ_0 and μ_1 constitutive constants, we have

$$\eta_1 = \mu_1. \tag{25}$$

The new variables are

$$y = t,$$
 $w = \mu_1 x + u(y),$ $E = v(y) - \frac{(u(y) + \mu_1 x)^3}{3\mu_1 \lambda^2} + \frac{A(x)}{\lambda^2},$ (26)

where A'(x) = c(x), u(y) must satisfy the equation $\mu_0\mu_1 - u' = 0$ and v(y) is arbitrary. In this case we obtain the following solution of system (7)–(8):

$$w = \mu_1(x + \mu_0 t) + a_1, \qquad E = v(t) - \frac{(\mu_1(x + \mu_0 t) + a_1)^3}{3\mu_1 \lambda^2} + \frac{A(x)}{\lambda^2}, \quad (27)$$

where a_1 is an arbitrary constant and v(t) is an arbitrary function.

Symmetry reduction 1.4. For $\alpha = 1$, c(x) arbitrary and $\mu(E) = \frac{\mu_0}{2\mu_1 U_0 + E}$, with μ_0 and μ_1 constitutive constants, we have

$$\eta_1 = \mu_1 w. \tag{28}$$

The new variables are

$$y = t$$
, $w = u(y) e^{\mu_1 x}$, $E = v(y) - \frac{u^2(y) e^{2\mu_1 x}}{2\mu_1 \lambda^2} + \frac{A(x)}{\lambda^2}$, (29)

where A'(x) = c(x).

In this case the function v is arbitrary and u must satisfy the equation $\mu_0\mu_1u - u' = 0$. The corresponding solution of system (7)–(8) is

$$w = e^{\mu_1(x+\mu_0 t)+a_1}, \qquad E = v(t) - \frac{e^{2(\mu_1(x+\mu_0 t)+a_1)}}{2\mu_1 \lambda^2} + \frac{A(x)}{\lambda^2}, \tag{30}$$

where a_1 is an arbitrary constant and v(t) is an arbitrary function.

Symmetry reduction 1.5. For $\alpha = 1/2$, c(x) arbitrary and $\mu(E) = \frac{\mu_0}{E}$, with μ_0 a constitutive constant, we have

$$\eta_1 = \frac{-U_0}{H_0} (x + \mu_0 t) + a_1, \tag{31}$$

where a_1 is an arbitrary constant.

The new variables are y = t, $w = -\frac{U_0}{2H_0}x^2 - (\frac{U_0\mu_0}{H_0}t - a_1)x + u(y)$,

$$E = v(y) + \frac{A(x)}{\lambda^2} - \frac{1}{4H_0^2\lambda^2} \left[\frac{U_0^2 x^3}{5} + \beta (U_0 x^4 - 4H_0 u(y)x^2) + \frac{4}{3} (\beta^2 - H_0 U_0 u(y))x^3 + 4H_0^2 u^2(y)x \right],$$

where A'(x) = c(x), $\beta = \beta(t) = \mu_0 U_0 t - a_1 H_0$, v(y) is an arbitrary function and u(y) must satisfy the equation

$$-\mu_0 a_1 H_0 + \mu_0^2 U_0 y + H_0 u' = 0.$$
(32)

The solution of (32) is given by

$$u(y) = \mu_0 a_1 y - \frac{\mu_0^2 U_0 y^2}{2H_0} + a_2,$$
(33)

where a_2 is an arbitrary constant. To simplify the final result for E, we set $a_2 = \frac{-H_0^2 a_1^2 + k_1}{2U_0 H_0}$, so k_1 is an arbitrary constant, and the corresponding solution of system (7)–(8) is

$$w = -\frac{U_0}{2H_0}(x + \mu_0 t)^2 + a_1(x + \mu_0 t) + \frac{-H_0^2 a_1^2 + k_1}{2U_0 H_0},$$

$$E = v(t) + \frac{A(x)}{\lambda^2} - \frac{1}{4H_0^2 \lambda^2} \left[\frac{U_0^2}{5} x^5 + U_0 \beta x^4 + \frac{2}{3} (3\beta^2 - k_1) x^3 + \frac{2\beta}{U_0} (\beta^2 - k_1) x^2 + \frac{1}{U_0^2} (\beta^2 - k_1)^2 x \right].$$
(34)

3.2. *Case* 2. $\tau \neq 0$

When $\tau \neq 0$, we may set, without loss of generality, $\tau(t, x, w, E) = 1$. We will apply the classical Lie algorithm to system (7)–(8), where we have eliminated w_t and E_t by using (10).

The corresponding determining system leads to the following symmetry operators depending on α , the mobility μ and the doping concentration *c*:

(1) For α , μ and *c* arbitrary,

$$Y = \frac{\partial}{\partial t}.$$
(35)

(2) For α arbitrary, $c = c_0$ and $\mu = \mu_0 \neq 0$, with c_0 and μ_0 constitutive constants,

$$Y = f(t)\frac{\partial}{\partial x} + \frac{\partial}{\partial t} - \frac{f'(t)}{\mu_0}\frac{\partial}{\partial E},$$
(36)

where f(t) is an arbitrary function.

(3) For α and μ arbitrary, while $c = c_0$, with c_0 a constitutive constant,

$$Y = a_1 \frac{\partial}{\partial x} + \frac{\partial}{\partial t},\tag{37}$$

where a_1 is an arbitrary constant.

(4) For $\alpha = 3/2$, $c = \frac{c_0}{(x+c_1)^4}$ and $\mu = \mu_0 E^{\frac{\mu_1 - 4}{3}}$, with c_0, c_1, μ_0 and μ_1 constitutive constants,

$$Y = \frac{x+c_1}{\mu_1 t+a_1} \frac{\partial}{\partial x} + \frac{\partial}{\partial t} + \frac{-2w}{\mu_1 t+a_1} \frac{\partial}{\partial w} + \frac{-3E}{\mu_1 t+a_1} \frac{\partial}{\partial E},$$
(38)

where a_1 is an arbitrary constant.

Let us observe that these symmetries are the classical ones found in [17].

Symmetry reduction 2.1. When c, α and μ are arbitrary the new variables for the symmetry operator (35) are of the form y = x, w = u(y), E = v(y). In this case the solutions we are able to find are stationary ones and system (7)–(8) reduces to the following system for the unknown u(y) and v(y)

$$(2\alpha U_0 u^{2\alpha - 1} u' + u^2 v + H_0 (u' u'' - u u''')) \mu = k_1, \qquad -c + u^2 + \lambda^2 v' = 0,$$
(39)

where k_1 is an arbitrary integration constant. We can obtain an ODE for v by solving the second equation in u and by substituting in the first equation.

For some special forms of c and μ , we are able to obtain particular solutions of system (39), and then of system (7)–(8).

(1) *Trigonometric solutions*

If $c(x) = \cos^2(x + a_1) + 2\lambda^2 U_0 \cos^{-2}(x + a_1)$ with a_1 a constitutive constant, $\alpha = 1$ and μ arbitrary, by setting $k_1 = 0$ in (39) we obtain the following solution for the drift–diffusion system:

$$w = \cos(x + a_1), \qquad E = 2U_0 \tan(x + a_1).$$
 (40)

Since the derivatives of the trigonometric functions can be expressed in terms of the sine and cosine functions it is also possible to find solutions of the form $w = \sin^n(x+a_1)$, $E = \sin^k(x+a_1)$, for $n, k \in \mathbb{N}$ by adequately choosing μ and c(x). Of course μ can become complicated if n, k are big numbers, for instance

• If $c(x) = \sin^2(x + a_1) + \lambda^2 \sin(2x + a_1)$ and $\mu(E) = \frac{k_1}{E^2 + 2\alpha U_0 E^{\alpha - 1/2} \sqrt{1 - E}}$, with k_1 and a_1 constitutive constants, a solution of system (7)–(8) is

$$w = \sin(x + a_1), \qquad E = \sin^2(x + a_1).$$
 (41)

• If $c(x) = \sin^2(x + a_1) + \lambda^2 \cos(x + a_1)$ and $\mu(E) = \frac{k_1}{E^3 + 2\alpha U_0 \sqrt{1 - E^2} E^{2\alpha - 1}}$, with k_1 and a_1 constitutive constants, we obtain

$$w = \sin(x + a_1), \qquad E = \sin(x + a_1).$$
 (42)

• If $c(x) = \sin^4(x+a_1) + \lambda^2 \sin(2(x+a_1))$ and $\mu(E) = \frac{k_1}{E^3 + 4\alpha U_0 \sqrt{E-E^2} E^{2\alpha-1} + 4H_0 \sqrt{E-E^2}}$, with k_1 and a_1 constitutive constants, we obtain the solution

$$w = \sin^2(x + a_1), \qquad E = \sin^2(x + a_1).$$
 (43)

(2) Hyperbolic solutions

• When $\alpha = 2$, μ arbitrary and $c = c_0$ with c_0 a constitutive constant, by choosing $k_1 = 0$ in system (39) we obtain the following solution:

$$w = \pm \sqrt{2c_0} \cosh\left(\frac{x+a_1}{2\lambda\sqrt{2U_0}}\right), \qquad E = \frac{-c_0\sqrt{2U_0}}{\lambda} \sinh\left(\frac{x+a_1}{\lambda\sqrt{2U_0}}\right), \tag{44}$$

where a_1 is an arbitrary constant.

• For $c(x) = \sinh^2(x + a_1) + \lambda^2 \sinh(x + a_1)$ and $\mu(E) = \frac{k_1}{E(E^2 - 1 + 2U_0\alpha(E^2 - 1)^{\alpha - 1/2})}$, with k_1 and a_1 constitutive constants, we obtain

$$w = \sinh(x + a_1), \qquad E = \cosh(x + a_1).$$
 (45)

• For $c(x) = a_1 e^x (\lambda^2 + a_1 e^x)$ and $\mu(E) = \frac{k_1}{E^3 + 2\alpha U_0 E^{2\alpha}}$, with k_1 and a_1 constitutive constants, we get

$$w = E = a_1 e^x. ag{46}$$

(3) Jacobian elliptic solutions

In some particular cases we are able to obtain cnoidal waves u(x) as solutions of (39).

• For
$$c(x) = cn^4(x + a_1, m) + \lambda^2 cn(x + a_1, m) dn(x + a_1, m)$$
 and

$$\mu(E) = k_1 E^{-1} [(1 - E^2)^2 - 4\sqrt{(1 - E^2)(1 - mE^2)} (H_0(1 + m(3E^4 - 6E^2 + 2)) + \alpha U_0(1 - E^2)^{2\alpha - 1})]^{-1},$$

with a_1 and m constitutive constants, we obtain the solution

$$w = cn^{2}(x + a_{1}, m), \qquad E = sn(x + a_{1}, m),$$
 (47)

where sn, cn, dn are the Jacobi elliptic functions [1] of parameter m. • For $c(x) = cn^4(x + a_1, m) - 2\lambda^2 sn(x + a_1, m)cn(x + a_1, m)dn(x + a_1, m)$ and

$$\mu(E) = \frac{\kappa_1}{E^3 - 4\sqrt{E(1 - E)(1 + m(E - 1))}(H_0(1 + m(3E^2 - 1)) + \alpha U_0 E^{2\alpha - 1})},$$

with a_1 and m constitutive constants, we obtain
 $w = cn^2(x + a_1, m), \qquad E = cn^2(x + a_1, m).$ (48)

Taking into account that sn(z, 0) = sin(z), cn(z, 0) = cos(z), sn(z, 1) = tanh(z) and $cn(z, 1) = dn(z, 1) = cosh^{-1}(z)$, the solutions (47) and (48) also give trigonometric and hyperbolic solutions of the system (7)–(8).

(4) Solutions in Wadati functions

С

The Wadati functions are functions of the form $W = \frac{d}{dx} \left(2 \arctan\left(\frac{n_1 \sin(n_2 x)}{n_2 \cosh(n_1 x)}\right)\right)$, where n_1, n_2 are Gaussian integers, i.e. complex numbers whose real and imaginary parts are integer. Since these functions can be written in terms of trigonometric or hyperbolic functions, some algebraic relations between the functions and their derivatives could be investigated. So, we will try to find some specific forms of *c* and μ for which we obtain solutions in Wadati functions. In the following special cases we obtain solutions of system (7)–(8):

• For

$$(x) = 36\left(\frac{3-2\cosh(2x)}{3\cosh(x)-4\cosh(3x)}\right)^2 + \lambda^2\sinh(x),$$

a complicated expression $\mu(E)$ can be obtained for which we have the following solution:

$$w = \frac{8\cosh(x)}{8\cosh(2x) - 7} - 2\operatorname{sech}(x), \qquad E = \cosh(x),$$
(49)

where w is a Wadati function with $n_1 = 3$, $n_2 = 2i$.

For

$$c(x) = 144 \left(\frac{2\cosh(2x) + \cosh(4x)}{8 + 9\cosh(2x) + \cosh(6x)}\right)^2 + 2\lambda^2\sinh(2x),$$

a complicated expression $\mu(E)$ can be obtained for which we have the following solution:

$$w = \frac{12(2\cosh(2x) + \cosh(4x))}{8 + 9\cosh(2x) + \cosh(6x)}, \qquad E = \cosh(2x), \tag{50}$$

where w is a Wadati function with $n_1 = 1$, $n_2 = 3i$.

(5) Weierstrass elliptic solutions

When $c = c_0$, with c_0 a constitutive constant, we can also find solutions in terms of Weierstrass elliptic functions $P(y, g_2, g_3)$. This class of functions satisfies the ODE $(P')^2 = 4P^3 - g_2P - g_3$. In fact, it is possible to check that here exists a complicated form for $\mu(E)$ such that we have a solution in Weierstrass elliptic functions of (39) and consequently the following solution of system (7)–(8):

$$w = \sqrt{c_0 - 2\lambda^2 P \sqrt{4P^3 - g_2 P - g_3}}, \qquad E = P^2.$$
(51)

Symmetry reduction 2.2. When the mobility and the doping profile are constants, from the symmetry operator (36) the new variables we obtain are y = x + a(t), w = u(y) and $E = v(y) + a'(t)/\mu_0$, where the functions u and v must satisfy the system

$$-2\alpha U_0 u^{2\alpha-1} u' - u^2 v + H_0 (u u''' - u' u'') = k_2, \qquad -c_0 + u^2 + \lambda^2 v' = 0,$$
(52)

 k_2 being an arbitrary integration constant.

In this case all the solutions w which we are able to find are traveling waves.

The constant solutions are particular solutions of the system (52) and the corresponding solution E of system (7)–(8) is not constant but it only depends on t:

$$w = \pm \sqrt{c_0}, \qquad E = \frac{-k_2}{c_0} + a'(t)/\mu_0.$$
 (53)

By solving the first equation of system (52) in v, derivating and substituting in the second equation, system (52) can be reduced to a single fourth-order ODE in u. This equation admits the symmetry operator $Z = \partial_y$ and can be reduced to a third-order equation.

If we choose $k_2 = 0$, by setting g' = v we can write system (52) as

$$\frac{\alpha}{1-\alpha}U_0u^{2\alpha-1} - ug + H_0u'' = k_3u,$$
(54)

$$-c_0 + u^2 + \lambda^2 g'' = 0, (55)$$

where k_3 an arbitrary integration constant. We have found the following particular solutions:

(1) For α arbitrary,

$$w = 0, \qquad E = \frac{c_0}{\lambda^2} (x + a(t)) + c_4 + \frac{a'(t)}{\mu_0},$$
 (56)

where a(t) is an arbitrary function.

(2) For $\alpha = 2$,

$$u = \pm \sqrt{2c_0} \cosh\left(\frac{y}{2\lambda\sqrt{2U_0}}\right), \qquad v = \frac{-c_0\sqrt{2U_0}}{\lambda} \sinh\left(\frac{y}{\lambda\sqrt{2U_0}}\right) \tag{57}$$

and the corresponding solutions of the drift-diffusion system are

$$w = \pm \sqrt{2c_0} \cosh\left(\frac{x+a(t)}{2\lambda\sqrt{2U_0}}\right), \qquad E = \frac{-c_0\sqrt{2U_0}}{\lambda} \sinh\left(\frac{x+a(t)}{\lambda\sqrt{2U_0}}\right) + \frac{a'(t)}{\mu_0}, \quad (58)$$

where a(t) is an arbitrary function. We observe that these solutions are a generalization of (44).

Symmetry reduction 2.3. In this case the doping profile is $c_0 = \text{constant}$ and the new variables that correspond to symmetry operator (37) are $y = x + a_1 t$, w = u(y) and E = v(y), where the functions u and v are solutions of the system

$$u^{2}a_{1} - 2\mu\alpha U_{0}u^{2\alpha-1}u' - \mu u^{2}v + \mu H_{0}(uu''' - u'u'') = k_{2}, \qquad -c_{0} + u^{2} + \lambda^{2}v' = 0$$
(59)

and k_2 is an arbitrary integration constant.

The solutions that correspond to this reduction are traveling waves.

By solving the second equation in u, differentiating and substituting in the first equation, system (59) can be reduced to a single fourth-order ODE in v. This equation admits the symmetry operator $Z = \partial_v$ and, by setting $z(v) = \frac{1}{v'(y)}$, can be reduced to a single third-order equation.

For some particular forms of the mobility we have found the following traveling wave solutions.

(1) If
$$\mu(E) = \frac{2(c_0 - \lambda^2 E)^2 (-k_2 + a_1(c_0 - \lambda^2 E))}{E(2c_0^3 + c_0^2 \lambda^2 (H_0 - 6E) + 6c_0 \lambda^4 E^2 - 2\lambda^6 E^3 - 2\alpha \lambda^2 U_0(c_0 - \lambda^2 E)^{1+\alpha})},$$

 $w = \pm \sqrt{c_0 - \lambda^2 e^{x + a_1 t}}, \qquad E = e^{x + a_1 t}.$
(60)

(2) If
$$\mu(E) = \frac{\lambda^2 (2k_2 + (\sqrt{1-E^2 - 1})a_1)}{E(\lambda^2 (\sqrt{1-E^2 - 1}) - 2^{-\alpha} u U_0 (1 - \sqrt{1-E^2})^{\alpha - 1})}$$
 and $c_0 = \frac{1}{2}$,
 $w = \sin\left(\frac{x + a_1 t}{4\lambda^2}\right), \qquad E = \sin\left(\frac{x + a_1 t}{2\lambda^2}\right).$
(61)

(3) If

$$\mu(E) = \frac{E\lambda^2 c_0^{\alpha+3}(-k_2 c_0 + a_1 \lambda^4 E^2)}{2\alpha c_0^3 \lambda^{4\alpha} U_0 E^{2\alpha} (c_0^2 - \lambda^4 E^2) + c_0^{\alpha} \lambda^6 E^4 (c_0^3 - 4c_0^2 H_0 \lambda^2 + 4H_0 \lambda^6 E^2)},$$
(62)

$$w = \sqrt{c_0} \tanh(x + a_1 t), \qquad E = \frac{c_0}{\lambda^2} \tanh(x + a_1 t).$$
 (63)

(4) If
$$\mu(E) = \frac{c_0^{\alpha^{+3}\lambda^2} E(a_1\lambda^4 E^2 - c_0k_2)}{\lambda^6 E^4 (4H_0 E^2 \lambda^6 - 4c_0^2 H_0 \lambda^2 + c_0^3) c_0^{\alpha} + 2\alpha \lambda^{4\alpha} U_0 E^{2\alpha} (c_0^2 - \lambda^4 E^2) c_0^3},$$

 $w = \sqrt{c_0} \coth(x + a_1 t), \qquad E = \frac{c_0}{\lambda^2} \coth(x + a_1 t).$
(64)

(5) If $\mu(E) = \frac{a_1}{E}$, $\alpha = 2$, $k_2 = 0$ and $y = x + a_1 t$, two classes of solutions can be found: (a)

$$= A sn(\gamma y, m), \qquad E = \frac{c_0}{\gamma \lambda^2} \mathbb{E}(am(\gamma y, m), m), \qquad (65)$$

where $E(\cdot, m)$ is the elliptic integral of second kind and parameter *m*, *am* is the elliptic amplitude [1], $A^2 = c_0 m$ and $\gamma^2 = \frac{U_0}{H_0} c_0$.

(b)

$$w = A cn(\gamma y, m), \qquad E = \frac{c_0}{(1-m)\gamma\lambda^2} E(am(\gamma y, m), m), \quad (66)$$

where $A^2 = c_0 \frac{m}{m-1}$ and $\gamma^2 = \frac{U_0}{H_0(1-m)}c_0$. (6) For $k_2 = c_0 a_1$ a long expression for μ can be found that leads to the following solution:

$$w = \sqrt{c_0 - 2\lambda^2 cn(x + a_1t, m)dn(x + a_1t, m)sn(x + a_1t, m)},$$

$$E = sn^2(x + a_1t, m).$$
(67)

Taking into account the properties of the elliptic functions, the solutions (65), (66) and (67) also lead to trigonometric and hyperbolic traveling wave solutions.

(7) Compactons. Compactons were introduced by Rosenau and Hyman [19] as a class of solitary wave solutions with compact support. In order to obtain a compacton solution f(y) for a differential equation, f must be a nonidentically null solution in a compact set Q, and f must be null when $y \notin Q$.

Let us observe that in (59), for $k_2 = 0$ and μ arbitrary, we can obtain the solution u = 0 and $v = \frac{c_0 y}{\lambda^2} + k_3$, with k_3 an arbitrary constant.

If $m \in \mathbb{N}$, $u = A \sin^m(\gamma y)$ for $y \in [0, k\pi/\gamma]$, and u = 0 elsewhere, then $u \notin C^{\infty}(\mathbb{R})$ but *u* have a jump discontinuity for the *m*-order derivative at the points y = 0 and $y = k\pi/\gamma$. It can be shown that for $m \ge 4$ the corresponding functions *u*, *v* are regular enough to be solutions for system (59), in the classical sense, by choosing an adequate function $\mu(|E|)$.

For instance, we can find a k-hump compacton in the following way.

If $\gamma > 0$ and we denote $Q = [0, k\pi/\gamma], k \in \mathbb{N}$, then a solution u, v of (59) is given by

$$u = \begin{cases} A \sin^4(\gamma \ y), & y \in Q \\ 0, & \text{elsewhere} \end{cases}$$
(68)

and

$$v = \begin{cases} \varepsilon \frac{c_0 s}{105\lambda^2 \gamma} \sqrt{1 - s^2} (48s^6 + 56s^4 + 70s^2 + 105), & y \in \left[0, \frac{k\pi}{\gamma}\right], \\ \frac{c_0}{\lambda^2} \left(y - \frac{k\pi}{\gamma}\right), & y > k\pi/\gamma, \\ \frac{c_0}{\lambda^2} y, & y < 0, \end{cases}$$
(69)

where $A^2 = \frac{128c_0}{35}$ and $s = \sin(\gamma y)$, with $\varepsilon = 1$ for $y \in Q$ and $|y - 2m\frac{\pi}{\gamma}| \leq \frac{\pi}{2\gamma}$ for $0 \leq m \leq \lfloor \frac{k}{2} \rfloor$ and $\varepsilon = -1$ elsewhere in Q; where $\lfloor x \rfloor$ indicates the greatest integer less than or equal to x.

It can be checked that $u \in C^3(\mathbb{R})$, $v \in C^8(\mathbb{R})$ and that u, v define a solution of (59) with $k_2 = 0$ for $y \notin Q$.

For the pair u, v, the mobility μ has the form

$$\mu = \begin{cases} \frac{a_1 s^3}{s^3 v + \varepsilon 8 \gamma \sqrt{1 - s^2} (3\gamma^2 H_0 + \alpha U_0 A^{2\alpha - 2} s^{8\alpha - 6})}, & y \in \left]0, \frac{k\pi}{\gamma}\right[, \\ \frac{a_1}{v}, & y \in Q, y = \frac{(2m+1)\pi}{2\gamma}, \\ \mu_1(v), & \text{elsewhere,} \end{cases}$$
(70)

where $\mu_1(v)$ is an arbitrary function of v. At y = 0 or $y = k\pi/\gamma$, $\sin(\gamma y) = 0$, u = 0and $\mu = 0$ because $8\alpha > 6$; therefore, the coefficient of u''' in (59) degenerates and the uniqueness of the solution is lost [18]. The functions u, v are smooth enough in order to satisfy (59) for $y \in Q$.

Symmetry reduction 2.4. Let us recall that in this case $c = \frac{c_0}{(x+c_1)^4}$, $\mu = \mu_0 E^{\frac{\mu_1-4}{3}}$ and $\alpha = 3/2$. By considering the symmetry operator (38), we must distinguish two cases: $\mu_1 \neq 0$ and $\mu_1 = 0$.

• If $\mu_1 \neq 0$, the new variables are $y = \frac{x+c_1}{(\mu_1 t+a_1)^{1/\mu_1}}$, $w = \frac{u(y)}{(\mu_1 t+a_1)^{2/\mu_1}}$, $E = \frac{v(y)}{(\mu_1 t+a_1)^{3/\mu_1}}$, where u(y) and v(y) must satisfy the system

$$\begin{split} u\{6v^{7/3}(2u+yu')+\mu_0v^{\mu_1/3}[6v^2u'+v(18U_0u'^2+u((\mu_1-1)v'+9U_0u''))\\ &+3(\mu_1-4)U_0uu'v']\}+\mu_0H_0v^{\mu_1/3}[(\mu_1-4)v'(u'u''-uu''')\\ &+3v(u''^2-uu'''')]=0,\\ -c_0+v^4(u^2+\lambda^2v')=0. \end{split}$$

This system can be reduced to a single, but complicated, ODE. If $\mu_1 = 3m$, $m \in \mathbb{Z}$, we have found the following particular solution

$$u = \frac{9\lambda^2 U_0 \pm \sqrt{c_0 - 36H_0\lambda^2 + 81\lambda^4 U_0^2}}{y^2},$$
$$v = \frac{6(-2H_0 + U_0(9\lambda^2 U_0 \pm \sqrt{c_0 - 36H_0\lambda^2 + 81\lambda^4 U_0^2}))}{y^3}$$

The corresponding solution of system (7)–(8) is

$$w = \frac{9\lambda^2 U_0 \pm \sqrt{c_0 - 36H_0\lambda^2 + 81\lambda^4 U_0^2}}{(x+c_1)^2},$$

$$E = \frac{6(-2H_0 + U_0(9\lambda^2 U_0 \pm \sqrt{c_0 - 36H_0\lambda^2 + 81\lambda^4 U_0^2}))}{(x+c_1)^3}.$$
(71)

We observe that the corresponding solution of the drift-diffusion system becomes a stationary solution.

• If $\mu_1 = 0$, the new variables are $y = (x + c_1)e^{-t/a_1}$, $w = u(y)e^{-2t/a_1}$, $E = v(y)e^{-3t/a_1}$ and the new system is

$$u(6vu'(a_1\mu_0v + yv^{4/3} + 3a_1\mu_0U_0u') + u(12v^{7/3} - a_1\mu_0(12U_0u'v' + v(v' - 9U_0u'')))) + a_1\mu_0H_0(-4v'(u'u'' - uu''') + 3v(u''^2 - uu'''')) = 0,$$
(72)

$$-c_0 + y^4(u^2 + \lambda^2 v') = 0.$$
(73)

We obtain the solution $u = \frac{\pm \sqrt{c_0}}{v^2}$, v = 0, that gives, as solution of the system (7)–(8),

$$w = \frac{\pm \sqrt{c_0}}{(x+c_1)^2}, \qquad E = 0.$$
 (74)

Another solution of (72)–(73) is given by

$$u = \frac{9\lambda^2 U_0 \pm \sqrt{c_0 - 36H_0\lambda^2 + 81\lambda^4 U_0^2}}{y^2},$$
$$v = \frac{6(-2H_0 + U_0(9\lambda^2 U_0 \pm \sqrt{c_0 - 36H_0\lambda^2 + 81\lambda^4 U_0^2}))}{y^3}.$$

The corresponding solution of (7)–(8) are also given by (71).

4. Qualitative analysis of some solutions

In this section, we study some qualitative aspects of several classes of the exact solutions of system (7)–(8) that we have found in the previous section. From a physical point of view, the most interesting solutions are *k*-hump compactons, kinks, soliton–antisolitons, kinks– antikinks, periodic solutions, etc. Apart from the physical interest of the solutions we have displayed in this paper, they can be useful for some applications because they provide examples of benchmark solutions for testing numerical codes for the quantum drift–diffusion model.

4.1. Solutions that depend on arbitrary functions

(1) When the mobility and the doping profile are constant and $\alpha = 2$, we have obtained the solution (58), where a(t) is an arbitrary function. The form of this class of solutions allows us to obtain solutions with a given behavior as *t* varies; for instance, by choosing a(t) periodic we get a periodic solution (58), for a fixed *x*. We can also choose the arbitrary function a(t) in such a way that the electric field is bounded for any *x*.

Let us observe that if the device has length L and it is represented by the set [0, L]; then the electric field satisfies the following boundary condition depending on the arbitrary function a(t):

$$E(0,t) = \frac{-c_0\sqrt{2U_0}}{\lambda}\sinh\left(\frac{a(t)}{\lambda\sqrt{2U_0}}\right) + \frac{a'(t)}{\mu_0}.$$
(75)

By integration on the interval [0, L], we get that the bias potential for getting such a solution is

$$\Phi_{\text{bias}}(t) = \Phi(L, t) - \Phi(0, t) = 2c_0 U_0 \left(\cosh\left(\frac{L+a(t)}{\lambda\sqrt{2U_0}}\right) - \cosh\left(\frac{a(t)}{\lambda\sqrt{2U_0}}\right) \right) - L \frac{a'(t)}{\mu_0}.$$
(76)



Figure 1. Representation of the stationary solution given by (47), with m = 1 and $a_1 = 0$ (graphics (*a*) and (*b*)). In graphics (*c*), the Wadati function *w* given in (50) is plotted.

If in (58) we choose a(t) = constant, then we obtain the stationary solution (44), where the mobility is arbitrary. Since $\mu = \mu(|E|)$, in this case, we must restrict our solution to an interval where *E* has a constant sign.

(2) When α = 2, c(x) = c₀ e^{∓ λ √2U₀} and the mobility μ is constant, we have obtained solution (24), where an arbitrary function u(t) appears. By choosing a suitable u(t) in (24), we can have E > 0 for any x, t; this happens, for instance, when u(t) = 1 - tanh(t) > 0, c₀ > 0. In another way, if we take u(t) periodic then the solution (24) is periodic in time.

4.2. Stationary solutions

We have found some interesting stationary solutions.

- (1) For m = 1, the solutions (47) reduce to $w = \cosh^{-2}(x + a_1)$, $E = \tanh(x + a_1)$; these functions are stationary and have soliton and kink shape, respectively. In figure 1(*a*) and 1(*b*) we plot these two functions for $a_1 = 0$; it is clear that E > 0 for x > 0. In figure 1(*c*) we have also shown the Wadati solution *w* given by (50). This can be considered as a two-soliton-like bound state.
- (2) When the mobility is arbitrary, $c = c_0$ and $\alpha = 2$, we have found the stationary solution (44). With the mobility arbitrary but in the isothermal case ($\alpha = 1$), we obtained the stationary solution (40) in the case $c(x) = \cos^2(x + a_1) + 2\lambda^2 U_0 \cos^{-2}(x + a_1)$.

4.3. Traveling waves

When the doping profile is constant, we have obtained several classes of traveling-wave solutions.

- (1) When α is arbitrary, the functions w and E given in solution (61) are sinusoidal waves and the functions given in solution (63) are kinks. We observe that in this last case the electric field is certainly positive when $x + a_1 t > 0$. In figure 2(*a*) we have plotted the trigonometric solution $w = \sin(\frac{x+a_1t}{4\lambda^2})$ given in (61) (with $\lambda = \frac{1}{\sqrt{2}}$, $c_0 = \frac{1}{2}$ and $a_1 = 2$). In figure 2(*b*) the kink function w given in (63) (with $c_0 = 1$ and $a_1 = 2$) is plotted.
- (2) When $\mu = a_1/E$, $\alpha = 2$, we have obtained the classes of solutions (65) and (66), with parameter *m*. In both cases the function *w* is a Jacobi elliptic function and *E* is an elliptic integral function. In figure 3 we have plotted the functions *w* and *E* given in (65) for m = 0.999, $c_0 = 2$, $a_1 = 2$, $H_0 = 0.0188$, $U_0 = 0.02$ and $\lambda = 1$. Let us observe that *w* is a squared traveling wave and *E* is a 'stair function', a bound state with infinity kinks. The cnoidal solution *w* in (66) is real for $c_0 > 0$ with m < 0 or m > 1 and has a sinusoidal or reciprocal sinusoidal shape, respectively.



Figure 2. Representation of the functions w given by (61) (a) and (63) (b), for $\lambda = 1/\sqrt{2}$, $a_1 = 2$, and $c_0 = 1/2$ (a) and $c_0 = 1$ (b).



Figure 3. Representation of the elliptic traveling wave solutions w and E in (65) with m = 0.999, $c_0 = 2$, $a_1 = 2$, $H_0 = 0.0188$, $U_0 = 0.02$ and $\lambda = 1$.



Figure 4. Representation of the soliton–antisoliton (*a*) and kink–antikink (*b*) structures that correspond to solution (67), $a_1 = 2$, $c_0 = 1$, $\lambda = 1$, m = 1. In the graphic (*c*) we plot the function *w* that correspond to m = 0.9 and gives a net of dromions–antidromions from (67).

(3) The functions w, E given in solution (67) are Jacobi elliptic functions, where $E \ge 0$, for $x, t \in \mathbb{R}$. In figure 4(*a*), 4(*b*) we have plotted the functions w and E for $a_1 = 2, c_0 = 1, \lambda = 1, m = 1$. We can observe that w leads to a soliton-antisoliton bound state localized with respect to $\sqrt{c_0} = 1$ and E leads to a kink-antikink structure.



Figure 5. Representation of the 2-hump compacton w, and its related function E, that correspond to solution (68)–(69), k = 2, A = 0.2, $\gamma = 2$ and $\lambda = 3$.

These solutions only transport energy. When m = 0.9, the corresponding w leads to a periodic net of dromions–antidromions, that is represented in figure 4(c).

(4) One of the most interesting solutions we have found is the k-hump compacton (68). Although solitons are exponentially localized, they have infinite tails that may interact for an infinite time with other solitons. They may be inadequate with the extremely small spatial scales that are used in quantum models. For these models, it is natural to search soliton-like solutions with a finite span, i.e. compactons. Consider a single compacton wave along a nanotube whose wavelength is the same as the diameter of the nanotube. Since almost no energy is lost this can lead to a very fast flow in the nanotube.

The functions w, E that correspond to (68), (69) are plotted in figure 5, with $k = 2, A = 0.2, \gamma = 2$ and $\lambda = 3$. Let us observe that the 2-compacton w leads to a bound state of two humps and E leads to an unbounded travel structure.

5. Conclusions

For the quantum drift–diffusion equation, we have found several new families of solutions that have not been considered before. To obtain the first reductions we have used the nonclassical method of symmetries. A qualitative analysis of some of these families of solutions has also been made. Several classes of coherent structures are displayed by some of the solutions: kinks, periodic nets of dromions–antidromions, solitons–antisolitons bound states, kink–antikink structures, etc. We have shown that the system admits a wide class of solutions w, E where w is a compacton.

Acknowledgments

We warmly thank Professor Juan Luis Romero for enlightening discussions. RT acknowledges the financial support from PRA (ex 60%) of University of Catania and from GNFM through the *Progetto Giovani 2008*. JR acknowledges the financial support of DGICYT project MTM2006-05031, the project P06-FQM-01448 and FMQ201 group from Junta de Andalucía.

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