Solitons in Superlattices: Multiple Scales Method

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Negative differential conductivity is one of the basic characteristics of superlattices. A self-trapped potential is used to describe the formation of electric field domains resulting from negative differential conductivity. The method of multiple scales, in which the electric field profile is separated into fast and slow spatial components, shows that the slowly varying component satisfies the nonlinear Schrödinger equation. The well-known soliton solutions of this equation provide a theoretical description of the electric field domains. The soliton solutions imply that solitons are observed as envelopes of the linearized wave functions that correspond to the electric field domains in semiconductor superlattices.

Solitons in Superlattices have attracted considerable attention in recent years. Superlattices are fascinating because the structures exhibit collective properties not shared by either constituent, and these properties can be controlled through variation of the structural parameters (Chen and Mills, 1987). Negative differential conductivity is one of the basic characteristics of superlattices. Negative differential conductivity can result in the formation of electric field domains. The time-dependent oscillations of the current in GaAs/AlAs superlattices subject to DC voltage bias have been found (Kwok *et al.*, 1995). For large values of the photoexcitation or doping, there is a stable formation of stationary electric field domains leading to the well-known oscillatory *I–V* characteristic (Grahn *et al.*, 1995).

It is well known that the fluctuation decays for positive differential conductivity and grows for negative differential conductivity. Negative differential conductivity leads to the growth of a small negative charge accumulation (Tian and Ma, 1997). The lower field upstream leads to an increased rate of feeding electrons into the accumulation layer, and the high-field downstream leads to a decreased rate of removal from there. The spatially homogeneous electron distribution then

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becomes unstable, and a travelling electron accumulation layer is formed. In this process, a higher electron density nucleates an accumulation layer. So the formation of the electron accumulation layer can be described by the self-trapped potential $\kappa |\psi(x, t)|^2$, where $\psi(x, t)$ is the electron wave function, $|\psi(x, t)|^2$ is the electron density, and κ is a real constant (Tian and Ma, 1998).

The electric field profiles can be separated into fast and slow components (Chen and Mills, 1987; Tian and Ma, 1998). The first of these varies on the scale of the individual layers of the superlattices and is similar to the Bloch functions in solid state physics. The second component varies on a much larger scale and acts as an envelope for the fast Bloch-like component.

In the present paper we use the self-trapped potential $\kappa |\psi(x, t)|^2$ to describe the formation of electron accumulation-layer domains in semiconductor superlattices under DC voltage bias. In order to find the solution for the slowly varying component of the field, we use the method of multiple scales (de Sterke and Sipe, 1988). We show that the slowly varying component satisfies the nonlinear Schrödinger equation, which has soliton solutions. This implies that electron accumulationlayer domains in semiconductor superlattices are a soliton phenomena.

The formation of electron accumulation-layer domains in semiconductor superlattices based on the negative differential conductivity can be described by the self-trapped potential $\kappa |\psi(x, t)|^2$. Then the Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 - V(x) + eFx - \kappa |\psi(x, t)|^2$$
(1)

where V(x) = V(x + a) is the periodic superlattice potential with period *a*, *e* is the electron charge, and *F* is the strength of the electric field.

The corresponding Schrödinger equation is

$$i\frac{\partial}{\partial t}\psi(x,t) + \frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) - Fx\psi(x,t) + \kappa|\psi(x,t)|^2\psi(x,t) = 0$$
(2)

in which we taken $\hbar = 2m = e = 1$.

The following transformations (Chen and Liu, 1976)

$$\psi(x, t) = \Phi(x', t') \exp\left(-iFxt - \frac{1}{3}iF^2t^3\right)$$

$$x = x' - Ft'^2$$

$$t = t'$$
(3)

bring Eq. (2) to

$$i\Phi_t + \Phi_{xx} + V(x)\Phi + \kappa |\Phi|^2 \Phi = 0$$
(4)

where x' and t' are denoted by x and t for simplicity.

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If the system is linearized ($\kappa = 0$), the solution is

$$\Phi_{\omega(k)}(x,t) = \phi_k(x) \ e^{-\iota\omega t} + \text{c.c.}$$
(5)

where $\phi_k(x) = u_k(x) e^{ikx}$, $u_k(x) = u_k(x+a)$ is Bloch function, and c.c. designates complex conjugation.

Now we investigate the nonlinear equation (4). We use the method of multiple scales. This general technique calls in the present problem for the introduction of different length scales, $x_{\alpha} = \mu^{\alpha} x (\mu \ll 1, \alpha = 0, 1, 2, ...)$, and time scales, $t_{\alpha} = \mu^{\alpha} t$. These new variables are considered to be independent. Under this condition, the first spatial and temporal derivatives can be written as

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x_0} + \mu \frac{\partial}{\partial x_1} + \mu^2 \frac{\partial}{\partial x_2} + \cdots$$
(6)

and

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \mu \frac{\partial}{\partial t_1} + \mu^2 \frac{\partial}{\partial t_2} + \cdots$$
(7)

from which expressions for higher derivatives follow straightforwardly. Similarly, the wave function Φ is written as a series

$$\Phi = \mu \Phi_1 + \mu^2 \Phi_2 + \mu^3 \Phi_3 + \cdots$$
 (8)

The Φ_i (i = 1, 2, 3, ...) are functions of all x_α and all t_α . In taking V(x) to be strictly periodic, we assume that it shows variation only on the smallest length scale ($\alpha = 0$), that is $V = V(x_0)$. Equations (6), (7), and (8) are now substituted into Eq. (4) and terms with equal powers of μ are collected.

As a first step we gather all terms proportional to μ and find

$$i\frac{\partial}{\partial t_0}\Phi_1 + \frac{\partial^2}{\partial x_0^2}\Phi_1 + V(x_0)\Phi_1 = 0$$
⁽⁹⁾

This is just the linear equation. It shows that nonlinearity plays no role on the fastest spatial and temperal time scales. From the analysis earlier in this section we know that the functions in Eq. (5) are solutions to this equation. However, Eq. (9) only contains the variables x_0 and t_0 so that Φ_1 can be written as

$$\Phi_1 = a(x_1, x_2, \dots; t_1, t_2, \dots) \phi_k(x_0) \ e^{-\iota \omega t_0} + \text{c.c.}$$
(10)

where $a(x_1, x_2, ...; t_1, t_2, ...)$ is an arbitrary function of the slow variables, and we refer to it as envelope function.

Then as the second step we consider all terms proportional to μ^2 and obtain

$$i\frac{\partial}{\partial t_0}\Phi_2 + \frac{\partial^2}{\partial x_0^2}\Phi_2 + V(x_0)\Phi_2 + i\frac{\partial}{\partial t_1}\Phi_1 + 2\frac{\partial}{\partial x_0}\frac{\partial}{\partial x_1}\Phi_1 = 0$$
(11)

In order to solve this equation we make the following ansatz for Φ_2 :

$$\Phi_2 = \sum_{k'} b_{k'}(x_1, x_2, \dots; t_1, t_2, \dots) \phi_{k'}(x_0) e^{-i\omega(k)t_0} + \text{c.c.}$$
(12)

where $b_{k'}(x_1, x_2, ...; t_1, t_2, ...)$ is a new set of envelope functions. Substituting Eq. (12) into Eq. (11), we find

$$\sum_{k'} [\omega(k) - \omega(k')] b_{k'} \phi_{k'}(x_0) + i \frac{\partial a}{\partial t_1} \phi_k(x_0) + 2 \frac{\partial a}{\partial x_1} \frac{\partial \phi_k(x_0)}{\partial x_0} = 0$$
(13)

Now we project onto the subspace spanned by the eigenfunction $\phi_k(x_0)$ (= $u_k(x_0)e^{ikx_0}$). The first term of Eq. (13) then vanishes and the following condition for envelope function $a(x_1, x_2, ...; t_1, t_2, ...)$ is found:

$$\left(i\frac{\partial}{\partial t_1} + 2\left\langle k \left| \frac{\partial}{\partial x_0} \right| k \right\rangle \frac{\partial}{\partial x_1} \right) a = 0$$
(14)

or

$$\frac{\partial a}{\partial x_1} = -\frac{1}{v_k(x_0)} \frac{\partial a}{\partial t_1} \tag{15}$$

where the orthogonality relations of Bloch functions were used, and

$$\frac{2}{i}\left\langle k \left| \frac{\partial}{\partial x_0} \right| k \right\rangle = v_k(x_0)$$

 $v_k(x_0)$ is the group velocity in the eigenstate $\phi_k(x_0)$. Let

$$z_1 = x_1 - \frac{2}{i} \left\langle k \left| \frac{\partial}{\partial x_0} \right| k \right\rangle t_1 = x_1 - v_k(x_0) t_1$$

It follows that the slowly varying function $a(x_1, x_2, ...; t_1, t_2, ...)$ cannot depend on x_1 and t_1 independently but only on their linear combination. This brings us to the important conclusion that, to this level of approximation, the envelope travels with the group velocity. This conclusion reflects the fact that the nonlinearity has not entered the discussion yet.

Now we finally collect all the terms proportional to μ^3 . It is only at this level that the nonlinearity explicitly enters the discussion. The result can be written as

$$\begin{bmatrix} i\frac{\partial}{\partial t_0} + \frac{\partial^2}{\partial x_0^2} + V(x_0) \end{bmatrix} \Phi_3 + \begin{bmatrix} i\frac{\partial}{\partial t_1} + 2\frac{\partial}{\partial x_0}\frac{\partial}{\partial x_1} \end{bmatrix} \Phi_2 + \begin{bmatrix} i\frac{\partial}{\partial t_2} + 2\frac{\partial}{\partial x_0}\frac{\partial}{\partial x_2} + \frac{\partial^2}{\partial x_1^2} \end{bmatrix} \Phi_1 + \kappa |\Phi_1|^2 \Phi_1 = 0$$
(16)

Like the analysis of Eq. (11), we use a similar ansatz as Eq. (12) for Φ_3 :

$$\Phi_3 = \sum_{k'} f_{k'}(x_1, x_2, \dots; t_1, t_2, \dots) \phi_{k'}(x_0) e^{-i\omega(k)t_0} + \text{c.c.}$$
(17)

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Substituting Eq. (17) into Eq. (16) and projecting onto the subspace spanned by $\phi_k(x_0)$, we find

$$i\frac{\partial b_k}{\partial t_1} + 2\sum_{k'} \left\langle k \left| \frac{\partial}{\partial x_0} \right| k' \right\rangle \frac{\partial b_{k'}}{\partial x_1} + i\frac{\partial a}{\partial t_2} + iv_k(x_0)\frac{\partial a}{\partial x_2} + \frac{\partial^2 a}{\partial x_1^2} \right. \\ \left. + \kappa |a|^2 a \int |\phi_k(x_0)|^4 \, dx_0 = 0$$
(18)

Now we analyze and rewrite Eq. (18) in a more practical form. To do so, we project Eq. (13) onto the space spanned by the remaining eigenfunctions $\phi_{k'}(x_0)(k' \neq k)$. Using the orthogonality relation of Bloch functions, we find an expression for $b_{k'}$ in terms of the envelope function $a(x_1, x_2, \ldots; t_1, t_2, \ldots)$. It reads

$$b_{k'} = \frac{-2\langle k' | \frac{\partial}{\partial x_0} | k \rangle}{\omega(k) - \omega(k')} \frac{\partial a}{\partial x_1}$$
(19)

It follows from this expression that the envelopes $b_{k'}$ travel with the group velocity as well. If we interpret z_1 as our (slow) spatial coordinate (in the frame moving with the group velocity), we look for solutions for which $\partial/\partial x_2 = 0$. And t_2 can be identified as the (slow) time. After some algebraic manipulations, the result is

$$i\frac{\partial a}{\partial t_2} + \left[1 - \sum_{k' \neq k} \frac{4|\langle k'|\frac{\partial}{\partial x_0}|k\rangle|^2}{\omega(k) - \omega(k')}\right] \frac{\partial^2 a}{\partial x_1^2} + \kappa |a|^2 a \int |\phi_k(x_0)|^4 dx_0 = 0$$
(20)

At last, it is reduced to the nonlinear Schrödinger equation:

$$i\frac{\partial a}{\partial t_2} + A\frac{\partial^2 a}{\partial z_1^2} + B|a|^2a = 0$$
(21)

where

$$A = 1 - \sum_{k' \neq k} \frac{4 \left| \left\langle k' \right| \frac{\partial}{\partial x_0} \left| k \right\rangle \right|^2}{\omega(k) - \omega(k')}$$
$$B = \kappa \int |\phi_k(x_0)|^4 dx_0$$

The coefficient B represents the effective nonlinearity seen by the envelope function. The nonlinear Schrödinger (NLS) equation and its solutions have been widely studied (Tian, 1998). One of the best known properties, of this equation is the existence of soliton solutions. The NLS equation (21) for real B has the soliton solution (Abdullaev, 1993)

$$a = \sqrt{\frac{2}{B}} 2\eta \operatorname{sech} 2\eta \left(\frac{z_1}{\sqrt{A}} + 4\mu t_2 \right) \exp\left(-2i\mu \frac{z_1}{\sqrt{A}} - 4i(\mu^2 - \eta^2)t_2 \right)$$
(22)

Here, η is the soliton amplitude, $v = -4\mu$ is its velocity.

In conclusion, we use the self-trapped potential to describe the formation of electric field domains resulting from the negative differential conductivity. The electric field profiles can been separated into fast and slow components. Using the method of multiple scales, we present the results that the slowly varying component satisfies the NLS equation (21). Its soliton solution implies that solitons are observed as envelopes of the linearized wave functions that correspond to the electric field domains in semiconductor superlattices. Experimentally, electric field domains appear at high doping densities. Self-sustained current oscillations occur in weakly coupled superlattices. Frequencies reach GHz regime, even at room temperature observation is possible (Kastrup *et al.*, 1997).

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