Multistability of conductance in doped semiconductor superlattices

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We use a simple nonlinear Kronig-Penney model to study multistability and discontinuity in the currentvoltage characteristics of doped semiconductor superlattices in a homogeneous electric field. Nonlinearity in our model enters through a self-consistent potential used to describe the interaction of the effective electrons with charge accumulation in the doped layers. We show that the process of Wannier-Stark localization is slowed down by the nonlinear effect in the doped layers, and that the shrinking and destruction of minibands in the superlattice by the nonlinearity is related to the occurrence of discontinuity and multistability in the transport of electrons.

The electric-field-induced Stark-ladder effect, Wannier-Stark (WS) localization, and the electro-optical properties and device applications in the semiconductor superlattices (SL), such as GaAs- $Al_xGa_{1-x}As$, have been studied extensively in recent years. $1-\tilde{6}$ Quantum effects become significant in such systems because the electron wavelength is of the same order as the superlattice constant. Recently, there has been renewed interest in the study of multistability and discontinuity in the current-voltage $(I-V)$ characteristic of doped semiconductor superlattices, both theoretically^{',} and experimentally. 9 The charge domain theory for multistability is based on the idea that the charges of the carriers cannot move continuously as the biased voltage is increased; instead, they accumulate in one well for a certain time and, for larger fields, move spontaneously to the next well. Microscopic theories so far have not been able to take a complete account of the quantum mechanical wave nature of the carriers.

As a step toward the direction of considering the wave nature of the carriers, we propose a simple quantum mechanical model based on self-consistent potentials, and study the transport of ballistic electrons in terms of transmissions of quantum mechanical waves in a SL heterostructure. We neglect the scattering of the waves by impurities and phonons. Our emphasis here is not to build a complete model that takes everything into account, but rather gain an insight into the nature of electronic wave coherence and interferences by considering the interwell coupling and the interactions of an electron with a self-consistent potential, while neglecting scattering and other effects. By solving a tunneling and transmission problem for the electrons in the quantum well (QW) heterostructure, we avoid making the usual assumption of strong barriers and weak interwell coupling. We demonstrate that multistability and discontinuity in the transport of carriers are related to the shrinking and destruction of the miniband structure by the nonlinearity in the doped layers. We assume, for simplicity, that the longitudinal and transverse degrees of freedom are decoupled, thus resulting in an effectively one-dimensional problem. The interaction of an electron with charge accumulation in a doped layer is represented by a nonlinear term, that is seen to arise from a self-consistent potential in that layer.

We consider a SL that consists of a square-well/squarebarrier semiconductor heterostructure; this is a model of conduction bands representing the mismatch between two component materials of the superlattice. We consider two different models for the location of the doped layers. In the first model we assume that the doped layers coincide with the quantum barriers, whereas in the second model the doped layers are located in the center of the QW's. Following Ref. 10, we write the self-consistent Schrodinger equation for $\psi(x, t)$, the wave function for an electron in the SL, in the absence of an external field, as

$$
i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) + \int W(t,t';x,x') |\psi(x',t')|^2 dt' dx' \right] \psi(x,t),
$$
\n(1)

where $V(x)$ is the periodic lattice potential and $W(t, t'; x, x')$ is a kernel describing the interaction of the electron with the electrons in the charged layers.

We are interested in the time-independent solutions, $\psi(x, t) = \psi(x) \exp(iEt)$, and by assuming that the kernel is time independent we have the integral part of Eq. (1) proportional to the stationary density of charges in the doped layers. If the size of these regions is much smaller than the spatial variations of $\psi(x)$, the integral part of Eq. (1) can be replaced by the summation of the average contributions of the localized charges inside the wells, i.e., $\sum_{n} \overline{W} b |\psi(x_n)|^2$, where b is the width of the layer and \bar{W} is the average kernel in the well. The latter is proportional to $e^2 n_e/C$, where e is

the electron charge, n_e is the charge density in the doped layer, and C is the capacitance of that layer. For simplicity, we assume that we have ultrathin doped layers and use δ -function type nonlinear barriers to represent the selfconsistent potentials; this is an approximation which makes it possible to obtain a closed form expression for the model. In order for the δ -function model to be qualitatively compatible with the original QW structure, we require that the δ -function strengths are equal to the average barrier height in a cell leading to the replacement of the integral of Eq. (1) with the sum $\sum_n \overline{W} b^2 |\psi(x)|^2 \delta(x - x_n)$. The problem then reduces to that of studying a Kronig-Penney type model with nonlinear terms.¹¹⁻¹⁴

When an external electric field is applied along the growth axis of the superlattice, the most fundamental change that the field makes is the breaking of the translational symmetry. The energy levels of neighboring wells are misaligned, resulting in a WS localization due to the turning-off of the resonant tunneling between consecutive wells. Wannier-Stark localization has been used to explain shifted absorption edges of photocurrent^{$1-3$} and widened gap regions absorption eages of protocurrent and whence S_{up} research in the transmission spectrum.¹⁴ In this case, the timeindependent Schrödinger equation for the electron in an external electric field \mathcal{E} , with energy E, and approaching a sample of N periodic potential barriers is

$$
-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \left[\sum_{n=1}^N g(\vert\psi\vert^2)\delta(x-x_n) - e\mathcal{E}x\right]\psi(x) = E \psi(x), \quad (2)
$$

where $g(|\psi|^2) = p[g_0 + g_2 | \psi(x)|^2]$, p is the potential strength, g_0 and g_2 are weight factors $(pg_2 = \bar{W}b^2)$, representing the linear and self-consistent nonlinear potentials, respectively, and $x_n = na$, where a is the lattice constant. We define a characteristic length $l(\mathcal{E}) = (\hbar^2/2me\mathcal{E})^{1/3}$, and a dimensionless parameter $\lambda(\mathscr{E}) = (2m/\hbar^2 e^2 \mathscr{E}^2)^{1/3}E$. It can be easily shown that in the linear case $(g_2=0)$, between two adjacent scatters, Eq. (2) is transformed into a Bessel equa*tion* of order $\frac{1}{3}$, whose solution is expressed as a combination of *Hankel functions* of the first and second kind.¹⁵ This solution is also valid in the general nonlinear case $(g_2 \neq 0)$ since the nonlinear term is localized; we thus have for the wave function between x_{n-1} and x_n ,

$$
\psi_n(z) = A_n z^{1/3} H_{1/3}^{(1)}(z) + B_n z^{1/3} H_{1/3}^{(2)}(z), \tag{3}
$$

where $H_{1/3}^{(1,2)}(z)$ are the *Hankel functions* of the first and second kind, respectively, and $z(x, \mathscr{E}) = \frac{2}{3} \lambda^{3/2} (\mathscr{E}) [1 + x/\lambda]$ $\lambda(\mathcal{E})l(\mathcal{E})$ ^{3/2}, is a dimensionless coordinate. The effect of nonlinearity is included through the amplitude coefficients A_n and B_n which will be determined subsequently through boundary conditions.^{12,13}

We calculate the transmission coefficient for an electron in a SL in the presence of an external electric field, and use Landauer's formula to obtain the corresponding conductance. In order to do that, we must find the wave amplitudes, (A_n, B_n) , of Eq. (3). Considering the continuity of $\psi(x_n)$ and the discontinuity of its derivative due to the δ function at $x=x_n$, a recurrence relation connecting (A_{n+1},B_{n+1}) with (A_n, B_n) is obtained as follows: ^{12–14}

$$
\mathcal{M}:\n\begin{cases}\nA_{n+1} = \left[1 + w_n(\left|\psi_n\right|^2) h_n^{(1)}/h_n^{(0)}\right] A_n + w_n(\left|\psi_n\right|^2) h_n^{(2)}/h_n^{(0)} B_n, \\
B_{n+1} = \left[1 - w_n(\left|\psi_n\right|^2) h_n^{(1)}/h_n^{(0)}\right] B_n - w_n(\left|\psi_n\right|^2) h_n^{(3)}/h_n^{(0)} A_n,\n\end{cases}\n\tag{4}
$$

where $w_n = (2ml/\hbar^2)(\frac{3}{2}z_n)^{-1/3}p[g_0+g_2]\psi_n(z_n)|^2]$ and all the h_n 's are products (or sum of products) of Hankel functions of z_n : $h_n^{(0)} = H_{1/3}^{(2)}(z_n)H_{-2/3}^{(1)}(z_n) - H_{1/3}^{(1)}(z_n)H_{-2/3}^{(2)}(z_n),$ $h_n^{(1)} = H_{1/3}^{(1)}(z_n)H_{1/3}^{(2)}(z_n), \qquad h_n^{(2)} = H_{1/3}^{(2)}(z_n)^2, \qquad \text{and} \qquad h_n^{(3)}$ $=H_{1/3}^{(1)}(z_n)^2$. When the self-consistent interaction of the electrons in the doped layers is absent, i.e., when $g_2=0$, then Eq. (4) becomes independent of amplitudes A_n and B_n , and it essentially represents a transfer-matrix-type of equation. We observe that by using the properties of the δ functions, the nonlinear Kronig-Penney problem of Eq. (2) is replaced by the simple, invertible nonlinear map \mathcal{M} of Eq. (4). In this map, iteration by one step is equivalent to scattering through a δ -function barrier. In order to analyze the properties of the map $\mathcal M$ and calculate the transmission coefficient T for the electrons in the presence of the field \mathscr{E} , we use the standard back-propagation approach, i.e., we fix the amplitude of the outgoing wave at site N and iterate backwards to find A_0 , the desired input amplitude. We vary the values of A_N and obtain the complete set of A_N 's that corresponds to a given A_0 . The transmission coefficient through the superlattice with N

doped layers is given by $T = |A_N|^2/|A_0|^2$, whereas using the loped layers is given by $T = |A_N|^2 / |A_0|^2$, whereas using the Landauer formula, ${}^{16,17} G = (2e^2/h)T(1-T)^{-1}$, we also obtain the conductance G for the SL.

In Fig. 1 we show the electrical conductance G as a function of the field strength $\mathscr E$ for various values of g_2 . In the linear case $(g_2=0)$ and for a moderate electric field, the wave function of the electrons inside each quantum well is localized (WS localization) and the transmission is reduced due to the field induced reduction of the resonant tunneling between adjacent wells. As the electric field increases, the electrostatic potential energy of the electrons in each QW is enhanced by the amount of ea&; if this value becomes comparable to ΔE_g , the energy gap between two minibands, enhancement in transmission is expected because of the inersubband resonant tunneling.¹⁸ In the case of many minibands this process of enhanced transmission repeats itself also at higher field values resulting in the oscillatory pattern of the continuous curves in Fig. 1. This oscillatory behavior is a manifestation of the competition between WS localization and the intersubband resonance-induced delocalization.

FIG. 1. The effects of nonlinearity is shown from the conductance-field $(G-\mathscr{E})$ diagrams. For small nonlinear parameter g_2 , the transimission and conductance curves are tilted and shifted; for large g_2 , multiple transmissions and conductions become possible. The energy is chosen in the third transmission band (see Fig. 2), but multistability is also observed at other energies. An arrow is used to indicate a location of discontinuity. Other parameters are given in the text. The absolute values are used for the field strengths.

We note that the delocalization effect is completely absent from a single band model. The effects of WS localization and the intersubband resonance-induced delocalization can be observed through photon absorption and luminescence.^{1,2,18}

In the case of weak nonlinearity ($g_2=0.05$ in Fig. 1), the oscillatory behavior of transmission coefficient and conductance in the field remains similar to the linear case. However, the left and right sides of each peak become asymmetric, which means that (a) the WS localization process is slowed down in the presence of nonlinearity in the doped layers, as shown by the smaller slopes of the increasing curves in Fig. 1; and (b) the widths of the minibands shrink in the presence of moderate nonlinearity, so that the intersubband resonances occur in a narrower range of field values, resulting in the rapid drop after T or G reaches a peak value. Finally, drastic changes are observed in the case of strong nonlinearity $(g₂= 0.25$ in Fig. 1). We notice that WS localization process is further slowed down in a increasing field, whereas the miniband structure is totally destroyed by the nonlinearity, resulting in abrupt changes in transmission and conductance, including the occurrences of discontinuity and multistability. In Fig. 1 we use $a=20$ Å, $N=40$, and $E=0.32$ eV (this energy is roughly at the center of the second miniband of the linear model). For the barrier strength, we use $p = 2.0$ eV Å; $g_2=0.05$ and 0.25, respectively, with $g_0=1.0-g_2$.

In Fig. 2 we plot transmission and gap regions in the energy-field parameter plane; the regions of multistability are distinguished from regions with single transmission states and gaps. First, we notice that transmission bands become narrower and move downward in the energy direction with an increasing field strength, and the first band dies out at a field \mathscr{E} > 2.2 kV/cm. Second, the two bands around energy $E=0.3$ eV are the result of the breaking of a single transmission band of a corresponding linear lattice (not shown) by nonlinearity. We can see that Fig. 1 ($E=0.32$ eV) is consistent with Fig. 2 as far as multistability is concerned. If we consider the fact that there is always a distribution in energy for the electrons, we need to calculate the transmission and

FIG. 2. Contour plot of multistability in the $E-\mathscr{E}$ parameter plane. The black regions represent gaps or unstable regions; the dark gray regions are stable transmission states without multistablility and the light gray areas are the multistable states. Multistable states in the third transmission band (largest in this figure) exhibit an oscillatory pattern.

conductance according to that distribution. However, when the deviation is not large, Fig. 2 indicates that the typical behavior shown in Fig. 1 of multistability should remain the same. We used $g_2=0.25$, and other parameters are the same as in Fig. 1.

A second model has been used to study the nonlinear effects in the presence of the field in. more detail. In this model the doped layers are placed in the middle of the QW's instead of the barriers. After we obtain the conductance G as in the case of Fig. 1, we use field strength $\mathscr E$ and sample length Na to obtain the voltage $V=N aE$, we then use Ohm's law to obtain the current, $I = GV$. The current-field characteristic diagram and possible sweep-up and sweepdown paths for this second model are presented in Fig. 3. We use the following parameters for numerical calculations in Fig. 3: for the barrier potential, $g_0 = 1.0$, $g_2 = 0.0$; and for the doped layers, $g_0 = 0.5$, $g_2 = 0.5$. The rest of the parameters are the same as in Fig. 1.

FIG. 3. The current-field characteristic for the second model. Possible sweep-up and sweep-down paths are shown as the field is either increased or decreased. The current values (small circles) are obtained by calculating the conductance under different fields. Parameters are given in the text. The absolute values are used for the field strengths.

To give some intuition on the physical aspects of the map of Eq. (4), we can use an asymptotic form for the solutions. For the parameters of interest, $z \ge 1$ for all the x's; thus we can use the asymptotic form of the Bessel functions,

$$
H_{\nu}^{(1,2)}(z) \approx \sqrt{\frac{2}{\pi z}} \exp\left\{\pm i \left(z - \frac{\nu \pi}{2} - \frac{\pi}{4}\right)\right\} ,\qquad(5)
$$

where ν is the order of the Hankel function. Equations (3) and (4) can be simplified by using Eq. (5), and the recursion relations can be written as

$$
\tilde{A}_{n+1} = \eta [1 + w_n(|\psi_n|^2)] \tilde{A}_n \n+ \eta w_n(|\psi_n|^2) \tilde{B}_n \exp\{-2ik(x_n)x_n\}, \n\tilde{B}_{n+1} = \eta [1 - w_n(|\psi_n|^2)] \tilde{B}_n \n- \eta w_n(|\psi_n|^2) \tilde{A}_n \exp\{2ik(x_n)x_n\},
$$
\n(6)

where $\eta = (z_n/z_{n+1})^{-1/6}$, $\tilde{A}_n = \sqrt{2/\pi} z_n^{-1/6} A_n \exp(i\theta)$, and $\overline{B}_n = \sqrt{2/\pi} z_n^{-1/6} B_n \exp(-i\theta),$ with $\theta = (2/3)\lambda^{3/2} - (5/12)\pi$. We observe that the kinetic energy of the electron in the field, and the wave number, $k(x)$, are an increasing function of x, $k(x) = k_0[1 + (1/4)\lambda^{-3/2}k_0x^2 - (1/24)\lambda^{-3}k_0x^3 + \cdots],$ with $k_0 = \sqrt{2mE/\hbar}$. The asymptotic solution is then written as

$$
\psi_n(x) = (z_n/z)^{1/6} \tilde{A}_n e^{ik(x)x} + (z_n/z)^{1/6} \tilde{B}_n e^{-ik(x)x} . \tag{7}
$$

This solution corresponds to two modified plane waves

propagating in opposite directions. We note that the effect of the doped layers is to introduce a periodic "nonlinear kick" in the system described by the map of Eq. (6).

We have demonstrated that the occurrence of multistability and discontinuity in the transport processes of electrons can be explained by introducing self-consistent potentials representing the nonlinear space charge effects due to electron accumulation in the doped semiconductor layers. We use a simple model in which the doped layers are assumed to be ultrathin and act as nonlinear "kicks" on the wave packets of electrons. The introduction of δ -function-type potentials is not essential in obtaining the multistable behavior in transmission. One of the advantages of this model is that a fully quantum-mechanical treatment can be applied without using an effective Hamiltonian. Comparing with the tight-binding model, which is good for weakly coupled QW heterostructure, our model inherently creates a series of minibands (multiple conduction subbands structure), while the interwell coupling of the wave functions of all the QW's is also taken into account. These couplings are important for tunneling and transmission of electrons. However, we should point out that our model does not take into account any scattering processes. This model can be easily modified to study other heterostructures in an electric field, such as a SL consisting of alternative $n-$ and p -type doped layers and modifications made by impurities and disorder.

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