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Inhomogeneous boundary effects in semiconductor quantum wires

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Abstract. Boundary effects play an essential role in determining the physical properties of semiconductor quantum wires. Additional features come into play when one considers inhomogeneous boundaries, i.e. wires whose widths are functions of distance along the length of the wire. We show that, in the adiabatic approximation (which assumes that the boundary potential fluctuation effects, or equivalently, the variations in the wire width, occur on a scale much larger than the inverse of Fermi wavelength), the boundary problem for a quantum wire is equivalent to a one-dimensional Schrödinger equation along the wire with: (i) an effective potential provided by the deviation from the homogeneous boundary and, (ii) a wave function coupled to the lateral direction. In the periodic boundary fluctuation case, the subbands of the system split into many mini-subbands, and become a useful system to test 1D band theory. When the boundary fluctuates randomly, there exists in each of the subbands a mobility edge, below which the electron states are localized. The localization of the tail states of the top populated subbands makes the conductance drop smoothly whenever the Fermi energy passes the bottom of a new subband. The theory explains the recent experiments of Smith and co-workers.

1. Introduction

Recent improvements in nano-fabrication techniques are continually reducing the size of semiconducting devices [1,2] to the point where one obtains a semiconductor wire with a width comparable to the Fermi wavelength (of the order of 10^3Å) of the electrons. Then the lateral electron states are quantized into subbands, usually with several subbands being populated. Very often, these semiconductor quantum wires were obtained using a high-mobility two-dimensional (2D) electron gas as the starting material upon which a laterally confined potential is imposed by various nano-fabrication techniques. The result is referred to as quasi-one-dimensional (Q1D) system.

To date, various experimental efforts [1,2] have been made toward exploring the new physics emerging from a study of these Q1D systems, such as quantum ballistic conductance, weak localization phenomena, the extreme strong depolarization effect of the intersubband resonance transition, and the abnormal conductance near the tail regions of the subbands. On the theoretical side [3–9] it is becoming clear that the inhomogeneity of the wire boundaries (or, in other words, the variation in width of the wires) plays an important role in understanding the new physics of the Q1D systems. For example, the weak localization phenomenon [3,6] in Q1D systems must

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be discussed in conjunction with boundary effects. Also, our calculation [7] of the multiple-parallel uniform quantum wire system, based on a conventional transport theory extended from the bulk system, shows that the conductance always has a sudden drop whenever the Fermi energy reaches the bottom of another subband if a wire of uniform width is assumed. This is true even when one considers the level broadening effect and the electron multi-subband screen effect. We will demonstrate later in this paper that the *sudden drop of conductance* will be smeared out once one considers *inhomogeneous boundary effects*. Our work is also stimulated by the interesting numerical study of Kumar *et al* [9] in which they have shown that a smooth boundary potential is obtained for a semiconductor quantum wire even when the confining gate on the wire gives rise to an abrupt square potential. This is significant, because it implies that the well known adiabatic theory (see section 2) is applicable to the discussion of the boundary effects for the semiconductor quantum wires.

The importance of the boundary (interface) effect for the quantum mechanically confined semiconductor system was first discussed in the study of the 2D systems [10–12]. There, the activated temperature dependence of the conductivity at low carrier densities is attributed to the localization of the electron states in the band tail regions due to *the random potential fluctuations at the interface*. This strong localization phenomenon was recently studied in the case of the semiconductor quantum wire by Nixon and Davis [8] in the context of the random fluctuation of the impurity potentials. On the other hand, at high carrier densities when there is more than one subband being populated for the quantum confined system, no general treatment exists in parallel to the above mentioned Mott–Stern theory [10, 12]. The property of the electron states in the case of multi-populated subbands is one of the main subjects of the present paper. In addition, we study the effects of variations in the wire width due to fluctuations in the boundary along the lateral direction. When the fluctuation is random, all the states near the bottom of each populated subband are localized. When the fluctuation is periodic, each subband will split into mini-subbands. A brief account of the present work has been previously reported [13].

In section 2, under the assumption that the adiabatic approximation is valid, we give an analysis of the boundary effect in Q1D systems, and show that it is equivalent to solving a 1D Schrödinger equation along the wire with: (i) an effective potential resulting from the deviation from the homogeneous boundary and (ii) a wave function coupled to the lateral direction. In section 3, the case of the random fluctuating boundary is studied. In section 4, we apply our results to discuss conductance near the subband tail region. Our results are summarized and discussed in section 5.

2. Formulation

Semiconductor wires are constructed by applying a gate voltage to a two-dimensional system to produce lateral confinement. The fluctuations in the potential mean that, in essence, we have to deal with a two-dimensional Schrödinger equation. However, in the adiabatic approximation (which assumes that the potential variation occurs on a length scale much greater than the Fermi wavelength), the problem can be reduced to an effective one-dimensional problem. In this section we show that, in the *adiabatic approximation*, the boundary fluctuation effects (which result in a variation in the wire width, which we take to be along the y-direction) on a Q1D system are equivalent to solving a 1D Schrödinger equation along

the wire with: (i) an effective potential provided by the boundary fluctuation; and (ii) a wave function coupled to the lateral direction of the wire (the x-direction). The basic idea is implicit in the work of Mott [12] on two-dimensional systems, carried out in the seventies. Recently, Glazman *et al* have explicitly used the adiabatic approximation to study the quantum ballistic transport of a microscopic constriction. It is our purpose here to use a similar approach to treat semiconductor wires of smoothly varying width. In particular, we stress that the *adiabatic approximation* is generally *applicable* to the Q1D systems where numerical study shows that a smooth potential is obtained even when the confining gate on the wire gives rise to an abrupt square potential [9].

The Schrödinger equation for an electron in a quantum wire with a lateral potential $V(x, y)$, has the form

$$\left[\frac{-\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right]\psi(x,y)=E\psi(x,y) \tag{1}$$

where, for simplicity, we have assumed that the electron has the same effective mass, m^*, along the x and y directions. In writing (1), we have assumed that in the absence of the lateral potential $V(x, y)$, the 2D system we are concerned with has extended states (see, for example, [12], p 107). This is a good approximation for the experiments of interest [1, 17] where the sample size is of the order of microns and the mobility is very high so that the localization length is several orders of magnitude larger than the characteristic length of the sample. For example, for a typical experimental situation [1, 17] the mean free path $\ell \approx 1.7\,\mu$m and $k_F\ell \approx 1.7 \times 10^2$ so that we can use the formula given by Mott ([12], p 110) to evaluate the localization length $L = \ell \exp(\pi k_F \ell/2) \approx 1.7 \exp(267)\,\mu$m which is clearly much larger than the sample size ($\approx 5\,\mu$m).

For an *ideal* sample, $V(x, y)$ is homogeneous along the wire (independent of x), and will be denoted as $V(y)$. In this case, equation (1) is separable, and it follows that it has the eigen-energy $\epsilon_{nk} = \epsilon_n + \hbar^2 k^2/2m^*$ and eigen-function $\psi_{nk}(x, y) = (1/\sqrt{L})e^{ikx}\xi_n(y)$, which satisfies

$$\left(\frac{-\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}+V(y)\right)\xi_n(y)=\epsilon_n\xi_n(y). \tag{2}$$

We note that, in the literature, the harmonic potential with $V(y) = \frac{1}{2}m^*\omega_0^2 y^2$ and the hard wall potential with $V(y) = 0$ for $|y| < d$ and $V(y) = \infty$ for $|y| > d$, are two typical models adopted for solving (2). In any case, we assume (2) is solvable.

For a real sample, one expects $V(x, y)$ has some fluctuation from $V(y)$ at each position of x while keeping the basic features of $V(y)$ adopted in the ideal model (2). For example, in the study of Glazman *et al* for the quantum ballistic transport of a microscopic constriction [4] an x-dependent well width $d(x)$ is introduced in the hard wall potential, where $V(x, y) = 0$ for $|y| < d(x)$. Similarly, for the harmonic potential, one can introduce an x-dependence characteristic frequency $\omega_0(x)$ so as to write $V(x, y) = \frac{1}{2}m^*\omega_0^2(x)y^2$.

We proceed, in a fashion pioneered by Born and Oppenheimer, by treating x as a parameter, so that it follows that for each x, there still exists a solvable lateral confinement equation similar to (2)

$$\left(\frac{-\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}+V(x,y)\right)\xi_n^{(x)}(y)=\epsilon_n(x)\xi_n^{(x)}(y) \tag{3}$$

where the symbol (x) reflects the fact that (3) is different from (2) only in the fact that some characteristic quantity (ω_0 for the harmonic potential and d for the hard well potential) is now a function of x. Using (3) and $\psi(x,y) = \psi_n \equiv \varphi(x)\xi_n^{(x)}(y)$, (1) can be rewritten in the form of a 1D Schrödinger equation:

$$\left(\frac{-\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} + \epsilon_n(x)\right)\psi_n = E\psi_n. \tag{4}$$

Equation (4) tells us that the boundary fluctuation problem of a Q1D system can be reduced to a 1D potential problem. For this latter problem, there exists a vast literature [12, 14] and so it can be readily handled. We note that the above formulation can equally be applied to the 2D boundary problem, where the variable x is replaced by 2D vector r. For a related study of the 2D problem see, for example, [15].

Even though (4) is formally a 1D potential problem, the actual solution of (4) is much more complicated due to the fact that the ψ_n in (4) is a 2D wave function with x and y very much coupled as seen by (3). The approximation involved in treating (4) as an effectively 1D potential problem is equivalent to the standard *adiabatic approximation* used in obtaining the wave equation for nuclear motion[16] in the molecular problem, and it requires that the change of $\xi_n^{(x)}(y)$ is smooth in the range of k_{Fn}^{-1}, where k_{Fn} is the Fermi momentum of the nth subband. We expect that this approximation is good particularly for quantum wires, since the actual confinement potential is calculated self-consistently. In fact, a smooth potential is obtained even when the confining gate on the wire gives rise to an abrupt square potential.[9] Therefore, in the following study we will treat (4) as an effective 1D Schrödinger equation while keeping in mind that the ψ_n has a 2D form.

When the boundary fluctuation is small so that the $\epsilon_n(x)$ in (3) and (4) deviates from the ideal value ϵ_n only slightly, it is more convenient to rewrite $\epsilon_n(x) = \epsilon_n + V_n(x)$, with $V_n(x)$ a fluctuation potential around ϵ_n. Then, equation (4) becomes

$$\left(\frac{-\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} + V_n(x)\right)\psi_n = (E - \epsilon_n)\psi_n. \tag{5}$$

Some comments on equation (5) are in order. First of all, for an electron in the nth subband ($E > \epsilon_n$) in the quantum wire, equation (5) shows that the nature of the electronic states along the wire is controlled by the quantity $V_n(x)$ which is related to the boundary fluctuation directly. Secondly, among the various possible forms of $V_n(x)$, three cases are of particular interest: (i) $V_n(x) \equiv 0$; (ii) $V_n(x)$ periodic; (iii) $V_n(x)$ random. The $V_n(x) = 0$ case is simply the ideal sample case, where from equation (5) one recovers the solution $E = \epsilon_{nk} = \epsilon_n + \hbar^2k^2/2m^*$.

When $V_n(x)$ is periodic, equation (5) effectively represents an electron with energy measured from ϵ_n moving in a 1D periodic potential $V_n(x)$. Assuming that $V_n(x)$ has an amplitude V_0 and a period a, then the original free electron energy dispersion along the x-direction (corresponding to an ideal homogeneous boundary) is broken into many mini-subbands having a mini-width and mini-gap of the order of $\pi^2\hbar^2/2m^*a^2$ and V_0, respectively. The above observation is very interesting in that by manufacturing an appropriate periodic boundary on a quantum wire, it opens up the possibility of testing many 1D band models experimentally. This is because the estimated mini-gap ($V_0 \sim 2\,\mathrm{K}$ if we use a harmonic potential model with $\omega_0 \sim 20\,\mathrm{K}$ and $V_0/\omega_0 \sim 0.1$) is in a range detectable by experiments.

It is interesting to note there is other evidence that the above subject is worth pursuing further. In a recent work, Kumar *et al* [9] have studied the detailed shape of the confined potential in the presence of a periodic perturbation to the width of the wire. Their self-consistent numerical calculation demonstrates that the effective potential well for the channel electron gas does indeed have a good sinusoidal shape as the high-wave-vector components of the gate roughness are found to be attenuated out. In other words, a simple periodically perturbed effective potential well may be achievable under the experimental conditions.

3. Strong localization near the bottom of subbands: randomly fluctuating boundary

We now study the randomly-fluctuating boundary case, where we assume the maximum fluctuating amplitude V_M of $V_n(x)$ is much less than the characteristic energy of the confinement potential. In this case, equation (5) effectively represents an electron in a one-dimensional random potential. The difference is that here the wave function ψ_n is a two dimensional quantity as defined by (3) and (4). It follows that the usual arguments concerning all the states of electrons in a one-dimensional random potential does not apply to the Q1D equation (5), and one can directly extend the Mott–Stern localization theory [10–12] for the 2D electron gas. We note that if we replace the x in (1)–(5) by a 2D vector r and $V_n(x)$ by $V_n(r)$ a 2D random potential, then (5) is a direct mathematical manifestation of Mott and Stern's idea that a randomly-fluctuating boundary potential is a source of the band tail localization. Moreover, since (5) is good for any value of n as long as $E > \epsilon_n$, it demonstrates that the Mott–Stern localization theory applies to all the subband tail regions for a quantum confined system. In other words, (5) tells us that near the bottom of each populated subband, the electron states in a semiconductor quantum wire are strongly localized ($k_F\ell \gtrsim 1$) in the random-fluctuation boundary model, and the energy range of the localized states is of the order of $V_M^{(n)}$ (the mobility edge).

In addition to the above general observation, the subband tail localization brings more new physics to the Q1D system. First of all, our finding of the localization in the subband tails implies that a random-fluctuation boundary can wipe out the divergence of the density of states originally existing in the free electron model. This is illustrated by figure 1, where one observes that with the tail region localization, the density of states is now well behaved. Secondly, our model indicates that for each value of electron energy E at $\epsilon_\ell < E < \epsilon_\ell + V_M^{(\ell)}$, there exist $\ell + 1$ degenerate states among which the states belonging to the top subband are localized (see the insert of figure 1). In the literature it is generally argued that extended and localized states cannot coexist at the same energy for a given configuration [12]. Since the semiconductor quantum wire is very often populated with several subbands and the electrons belonging to different subbands have different symmetry properties, what we have presented here is a first example of the possible coexistence of the extended and localized states at the same energy with different symmetry in a quantum confinement. Thirdly, the discussion of the boundary condition of the semiconductor quantum wire is practical in the sense that it is more easily controlled experimentally than that of the 2DEG, where a detailed knowledge of the interfacial potential is generally lacking [11].

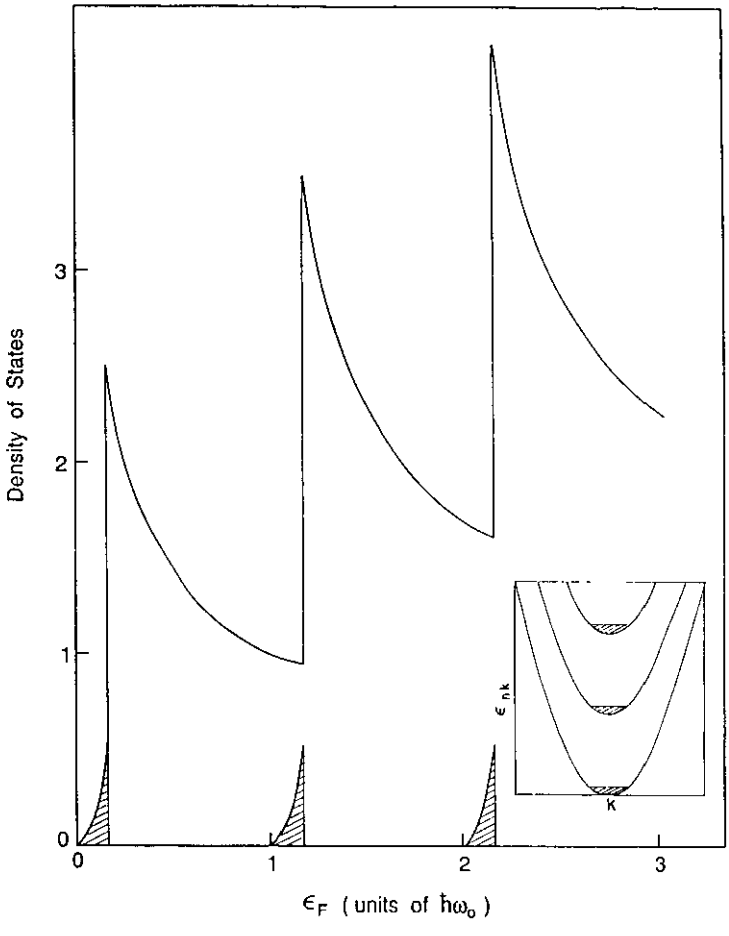

Figure 1. Density of states for electrons in a semiconductor quantum wire with a randomly-fluctuating boundary using the harmonic potential model. The suppression of the density of states near $\epsilon_F/\hbar\omega_0$ of integer values is due to the Anderson localization in the subband tails as indicated by the shaded areas in the insert for the energy ϵ_{nk} versus wave vector k.

4. Application: conductance near the subband tail region

Recently, in their transport measurements on a device consisting of a grating of multiple parallel quantum wires (MPQW) extending from source to drain, Ismail *et al* [17] have identified interesting negative differential conductance in the subband tail region. It is stressed by the authors that the advantage of having a large number of wires in parallel is to average out the universal conductance fluctuations and weak localization effects, which are caused by randomly distributed impurities. In a subsequent theoretical study of the subband effect on the quantum transport of MPQW, using the generalized quantum Langevin equation approach [7] we obtained a fairly good fit to the experimental data for the conductance (see the insert of figure 2). The only unsatisfactory part is in the subband tail region where the theoretical value

of the conductance always has a sudden drop whenever the Fermi energy reaches the bottom of another subband (even in the case where the level broadening effect and the electron multi-subband screen effect are included), while the experimental curve only shows a very smooth change. Here we show qualitatively that once we include the subband tail localization effect due to the random-fluctuation boundary discussed in the previous section, the sudden drop of conductance will be smeared out.

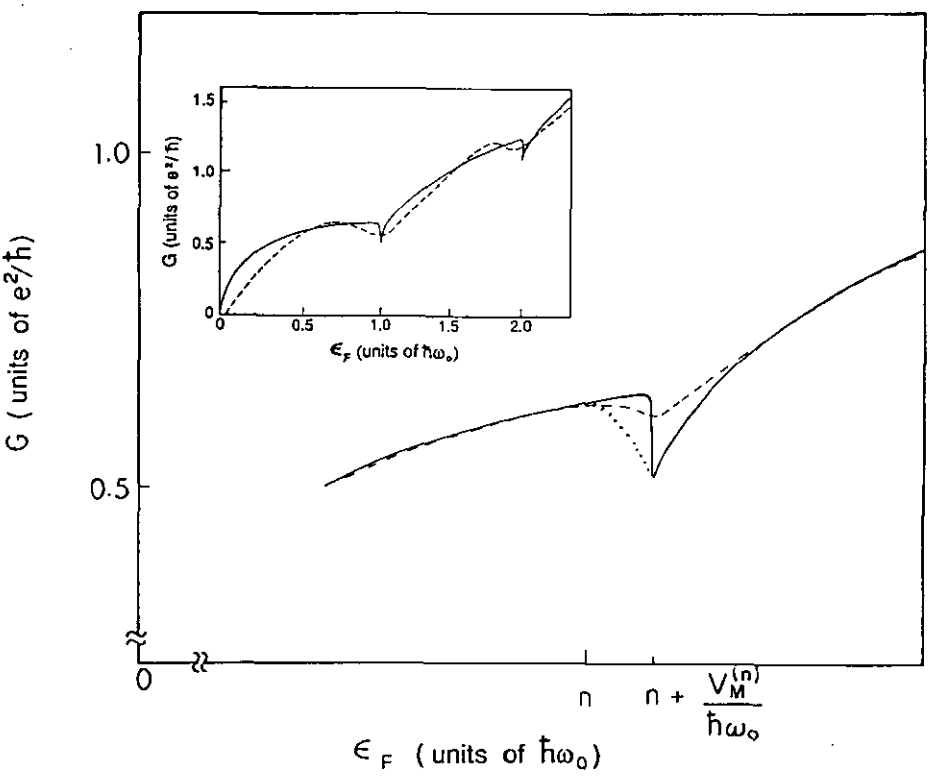

Figure 2. Schematic picture for the conductance G versus Fermi energy ϵ_F near the tail of the nth subband for a multiple parallel quantum wire with random boundary fluctuation and harmonic confinement potential model (with ω_0 the characteristic frequency). Full line: $T = 0$, with a mobility edge $V_M^{(n)}$ but neglecting the influence of the localized states on the conduction. Dot (dashed) line: $T = 0$ ($T \neq 0$), and including the contribution of the localized states. The inset is the theoretical result (full line) of [7] for a sample with homogeneous boundary as compared with the experimental data (dashed line).

The physical mechanism can be understood as follows. When the Fermi energy increases so as to reach the bottom of another subband, there appear two kinds of electrons at the Fermi level, one is in a *localized* state (which arises from the randomly-fluctuating boundary) in the *top* subband and the *other* is in an *extended* state in the lower subbands. At $T = 0$, the presence of the localized states will reduce the conductance of the system through the process of tunnelling and trapping, both of which depend on the number of the available localized states. This decreasing trend in the conductance is kept as long as the Fermi energy is below the mobility

edge of the top subband. After ϵ_F passes the $V_M^{(n)}$, all the states at ϵ_F are extended, and the conductance of the system recovers the metallic increasing behaviour.

The mathematical model for the conductance G in the above described region ($\epsilon_n \leqslant \epsilon_F \leqslant \epsilon_n + V_M^{(n)}$) can be formulated by using the following facts: (i) at the two end points $G_0 \equiv G(\epsilon_n)$ and $G_M \equiv G(\epsilon_n + V_M^{(n)})$, the conductance can be evaluated by the usual conductance calculation scheme for the extended states; (ii) in between, G decreases.

First, we qualitatively discuss the $T = 0$ situation. Because the increase of the number of the localized states is proportional to $\sqrt{\epsilon_F - \epsilon_n}$ for a 1D subband, we will *assume* that G is proportional to $\sqrt{\epsilon_F - \epsilon_n}$. It follows then that

$$G(\epsilon_F) = (G_0 - G_M)\left(1 - \sqrt{\frac{\epsilon_F - \epsilon_n}{V_M^{(n)}}}\right) + G_M \qquad 0 \leqslant \epsilon_F - \epsilon_n \leqslant V_M^{(n)} \tag{6}$$

where G_0 and G_M are to be evaluated by some known conductance formalism for the extended states. The dotted line in figure 2, gives (6) for the nth subband for a MPQW, where the values of G_0 and G_M are taken from our previous theoretical calculation (see inset of figure 2) for the homogeneous boundary system. Specifically, we take for G_M the value of G at the dip and we assume $V_M^{(n)}/\hbar\omega_0 \ll 1$ so that G_0 takes a value on the shoulder next to that dip. As can be seen from the figure, at $T = 0$ once the localization effect of the band tail states is taken care of, the conductance changes smoothly with ϵ_F except at the point $\epsilon_F = \epsilon_n + V_M^{(n)}$, which is still at variance with the experimental data (see inset of figure 2). Therefore, a finite-temperature theory for the localization effect in the MPQW is needed.

In the following we include the thermal effect by considering the contribution of the localized states to the conductance. According to the Mott theory [12] at $T \neq 0$ and $\epsilon_F - \epsilon_n < V_M^{(n)}$, the localized electrons below ϵ_F can be thermally activated by hopping into a nearby state above ϵ_F. As stated earlier, we consider our Q1D system has a 2D wave function, as a consequence of which it can be treated by the Mott–Stern 2D theory [10–12] of band tail localization. Therefore, for the Q1D system we follow exactly Mott's treatment of hopping conductance [12]. First we set up the hopping functional followed by finding the optimum hopping distance. For a 1D hopping system with hopping range R, the density of states per unit energy range is $2RN(\epsilon_F)$, where $N(\epsilon_F)$ is the density of states at ϵ_F. The inverse of this quantity is the activation energy for the hopping process through the distance R,

$$\Delta E = \frac{1}{2RN(\epsilon_F)}. \tag{7}$$

The hopping functional is defined as

$$F(R) \equiv e^{-2\alpha R - \Delta E/k_B T} \tag{8}$$

where ΔE is defined by (7) and $1/\alpha$ is the decay length of the localization wave function. From (7) and (8), the optimum hopping distance is determined by solving $\partial F/\partial R = 0$, which gives

$$R = (4\alpha N(\epsilon_F) k_B T)^{-1/2}. \tag{9}$$

Next, substituting (9) for the R in (8), we obtain the hopping probability and the conductance for the localized electrons in the top populated subband

$$G_L = G_0 \exp\left(-\sqrt{\frac{T_0}{T}}\right) \tag{10}$$

where G_o is a temperature-independent prefactor, and

$$T_0 = \frac{4\alpha}{N(\epsilon_F)k_B} \tag{11}$$

with α^{-1} the decay length of the localized wave function, and $N(\epsilon_F)$ the density of states at ϵ_F. We note the $T^{-1/2}$ law identified by (10) is also obtained by Shante and Varma [18] in a different approach for a parallel chain system with small disorder so that electronic wave functions extend over several sites.

Our estimate for T_0 of (11) is carried out in the following way. First, we assume that after ϵ_F passes the mobility edge $V_M^{(n)}$, all the band tail states have the same value of $\alpha = \alpha_0$. Since we are interested only in the contribution of the localized states to the conductance, the density of states in this case is roughly

$$N(\epsilon_F) \approx \frac{\sqrt{2m^* V_M^{(n)}}}{\hbar(\epsilon_F - \epsilon_n)} \qquad \epsilon_F - \epsilon_n > V_M^{(n)}. \tag{12}$$

Using (11), (12) and $\alpha = \alpha_0$, one obtains

$$T_0 = \begin{cases} T_\epsilon \dfrac{V_M^{(n)}}{\epsilon_F - \epsilon_n} & 0 < \epsilon_F - \epsilon_n < V_M^{(n)} \\ T_\epsilon \dfrac{\epsilon_F - \epsilon_n}{V_M^{(n)}} & \epsilon_F - \epsilon_n > V_M^{(n)} \end{cases} \tag{13}$$

where T_ϵ is defined by

$$T_\epsilon = \left(\frac{8\alpha_0^2 \hbar^2 V_M^{(n)}}{m^*}\right)^{1/2}. \tag{14}$$

In addition, the $0 < \epsilon_F - \epsilon_n < V_M^{(n)}$ part of (13) is obtained as follows. When the Fermi energy is below the mobility edge ($0 < \epsilon_F - \epsilon_n < V_M^{(n)}$), it is known [12] that α has a power law dependence on the energy,

$$\alpha = \alpha_0 \left(\frac{V_M^{(n)}}{\epsilon_F - \epsilon_n}\right)^\eta \qquad 0 < \epsilon_F - \epsilon_n \leqslant V_M^{(n)} \tag{15}$$

where by definition, $\alpha = \alpha_0$ at $\epsilon_F - \epsilon_n = V_M^{(n)}$. The density of states for this case is roughly

$$N(\epsilon_F) \approx \frac{\sqrt{2m^*(\epsilon_F - \epsilon_n)/\hbar}}{V_M^{(n)}}. \tag{16}$$

Substituting (15), (16) into (11), and assuming $\eta = \frac{1}{2}$, we obtain the $0 < \epsilon_F - \epsilon_n < V_M^{(n)}$ part of (13). We note that (13) is chosen by simply noticing the fact that at $\epsilon_F - \epsilon_n < V_M^{(n)}$, G_L increases with ϵ_F because it becomes harder for the hopping of the localized states once the ϵ_F passes the mobility edge $V_M^{(n)}$. We stress that the use of approximation (13), even though very crude, makes the physical process described by (10) much clearer. By definition, the T_ϵ in (13) is simply the value of T_0 at $\epsilon_F = \epsilon_n + V_M^{(n)}$, which can be easily estimated once the form of the confinement potential is known. For example, in the harmonic potential model $V(y) = \frac{1}{2}m\omega_0^2 y^2$, with $b = \sqrt{\hbar/m\omega_0}, \alpha \sim b^{-1}$, from (14) one has

$$k_B T_\epsilon = 4\sqrt{\frac{\hbar\omega_0 V_M^{(n)}}{2}}. \tag{17}$$

If we take $V_M^{(n)} \sim 10^{-1}\hbar\omega_0$, and $\hbar\omega_0 \approx 2\,\text{meV}$, then $T_\epsilon \sim 10\,\text{K}$.

At $T \neq 0$, the total conductance of the MPQW consists of the contributions from the extended states and the localized states. Assuming that the temperature dependence of the extended states contribution to the conductance is not very sensitive at $k_B T \ll \hbar\omega_0$, and the localized states contribution is the main temperature effect, the conductance (10) can then be simply added to the $T = 0$ conductance. Since our attempt here is to clarify the basic physical process for the transport in the band tail region and since the theory presented here depends on a choice of some unknown parameters, no detailed fit between our theory and experiments will be attempted in this paper. Instead, we will only draw a schematic picture to demonstrate that the theory presented here can explain the related experimental data. In figure 2 we plot G versus ϵ_F near the tail region of the nth subband for a MPQW with randomly fluctuating boundary and harmonic confinement potential. The figure shows that for a MPQW with randomly fluctuating boundary, because of the combined effects of the trap-tunnelling and the hopping from the localized states, once ϵ_F reaches the bottom of a new subband, the conductance at $T \neq 0$ changes smoothly. It drops first and then increases after ϵ_F passes the mobility edge of that subband. This explains the experimental results (dashed line in the inset of figure 2) that the conductance of MPQW has many saddles in consecutive order when sweeping the substrate voltage (which controls the ϵ_F) to the sample.

5. Conclusions

We have shown in this paper that, in general, the inhomogeneous boundary effects of a semiconductor quantum wire can be studied by reducing the problem to an effective 1D Schrödinger equation (4) along the wire. In that equation, the deviation from the homogeneous boundary is represented by a position- and subband-dependent effective 1D potential $\epsilon_n(x)$, and the wave function ψ_n is a two-dimensional quantity. This ψ_n is also effectively one-dimensional in the adiabatic approximation, and then the motion of electrons is reduced to a 1D potential problem (see (5)), with a potential provided by the deviation from the homogeneous boundary. When the boundary of the wire varies periodically then the original free electron energy dispersion along the x-direction (corresponding to an ideal homogeneous boundary) is broken into many

mini-subbands. As a result, a quantum wire manufactured with a periodic boundary should be an interesting system to test the 1D band model experimentally.

When the boundary of the wire varies randomly, we argue that, near the bottom of each populated subband, the electron states are strongly localized due to Anderson localization. This is a direct extension of the Mott–Stern localization theory of the 2D electrons to the Q1D multi-subband system. In particular, we identify some new features of the Q1D subband tail localization: (i) the elimination of the divergence of the density of states originally present in the homogeneous boundary model, (ii) the coexistence of extended and localized states in the same energy region but in different subbands. Also, we apply our theory to explain the recent experimental results of Smith *et al* [1] for the multiple parallel quantum wires, where many smooth saddles were observed consecutively in the conductance curve when sweeping the substrate voltage applied to the sample.

The transport theory presented in this paper for the semiconductor quantum wires is based on a physical picture of all the electronic states along the wire being extended except that those in the tail region (defined by the mobility edge) of each subband are localized. When the electron states are extended, and when the mean free path as well as the inelastic scattering length are much smaller than the sample length, the conventional transport theory is then applied to treat the quantum effect due to the presence of multi-subbands. After including the band tail localized states, our theory is in semi-quantitative agreement with the experimental results.

Recently, there have appeared other attempts [19, 20] to explain the same experimental results of [17] from a different perspective. In [19] starting from a localized picture and performing a numerical calculation, the conductance drop immediately after a new subband is populated, is associated with a decrease of the electron localization length. Similar to the present work and the experimental results of [1], smooth dips in the conductance versus ϵ_F plot, are identified near the region of the opening of a new subband. Unfortunately, no comparison with experimental results is available in [19]. Nevertheless, it is very interesting and our approach and that [19] give similar results even though two different approaches are used.

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