Magnetotransport in corrugated quantum wires

Anna Grincwajg* and David K. Ferry
Center for Solid State Electronics Research, Arizona State University, Tempe, Arizona 85287-6206
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The magnetoresistance of ballistic quantum wires with periodically modulated width has been calculated. We find that the negative magnetoresistance peak persists approximately up to 0.1 T, which is two orders of magnitude larger than in single quantum dots. Our results are in good agreement with recent experiments. We believe that the wide peak is a manifestation of a weak localization effect, arising from multiple backscattering and resonances among the segments of the corrugated wire. The weak localization effect is not sensitive to the period of corrugation, nor to the wire width, as long as the number of propagating modes is large. As random disorder is introduced, and the system approaches the diffusive transport regime, the wide negative magnetoresistance peak disappears. [S0163-1829(97)00607-3]

I. INTRODUCTION

Advances in semiconductor fabrication technology during the past decade have made it possible to create microstructures with dimensions comparable to the electron wavelength, such as quantum point contacts, quantum wires, and quantum dots.[1] A characteristic feature of these systems is the importance of interference effects between multiply scattered electron waves. Typical examples of interference effects that have been widely investigated are conductance fluctuations and weak localization. Both of these effects have been extensively studied experimentally and theoretically in diffusive systems, where electron scattering is mainly due to randomly positioned impurities.[2–6] However, if a system is ballistic, scattering will only take place at the geometrical boundaries of the structure, resulting in a new type of interference effects. One expects that interference effects resulting from geometry-induced scattering will contain features that depend on the actual geometry. The analog of conductance fluctuations and weak localization has recently been observed in ballistic cavities. One of the issues being discussed is how the corresponding classical motion, which may be chaotic or regular depending on the cavity geometry, influences the quantum-mechanical properties.[7–13]

In this work we focus on a different, but closely related aspect of how the microstructure geometry governs interference effects. We study the magnetotransport in corrugated ballistic quantum wires, making connection to some very recent experiments. Ochiai *et al.* have measured the magnetoresistance of ballistic quantum wires with periodically modulated width.[14] The wires were fabricated from the two-dimensional (2D) electron gas in a GaAs/Al$_x$Ga$_{1-x}$As heterostructure. Surprisingly, the negative magnetoresistance peak was found to persist to much higher field strengths than in single quantum dots,[8–11] the difference being roughly two orders of magnitude. We have performed numerical calculations to model the experiment and find good agreement, especially in the weak-field regime. The calculated negative magnetoresistance exhibits a peak, persisting approximately up to 0.1 T. We believe that this is a manifestation of a weak localization effect, arising from multiple backscattering and resonances among the segments of the corrugated wire. To our knowledge, this effect has not been discussed in the literature before. The phenomenon is a beautiful example of how the geometry totally dominates interference effects in ballistic structures.

An early experiment on a quantum wire with modulated width was performed by Kouwenhoven *et al.*[15], who studied a sequence of 15 quantum dots defined in a GaAs/Ga$_x$Al$_{1-x}$As heterostructure. The experimental data suggested the formation of a miniband structure in the periodic 1D crystal. An extensive theoretical investigation of conductance quantization in a corrugated quantum wire was later presented by Leng and Lent.[16] The authors showed that the conductance is quantized, in a fashion similar to the case of a single quantum point contact, but the quantization plateau index is not a monotonically increasing function. A band-structure calculation of the channel showed that the number of propagating modes is given by the number of Bloch bands with positive group velocity at a given energy. As a result, the conductance steps up and down with energy.

We cannot expect to find this type of conductance quantization in the present work, since the transport regime we are interested in is very different from the one considered in Refs. 15 and 16. In Ref. 15 the energy region allowed for only one propagating mode, and in Ref. 16 typically up to four propagating modes were considered. However, in the work of Ochiai *et al.*,[14] which we are modeling, the number of propagating modes is typically 50. Therefore, mode mixing will completely wash out the conductance steps, as will happen in any nonuniform quantum wire of this size. Consequently, the type of magnetotransport properties that we focus on in the present work differ strongly from the ones considered in Refs. 15 and 16.

II. THE MODEL AND METHOD

Our model geometry is taken to reflect the experimental structure of Ochiai *et al.*,[14] and is shown in Fig. 1. Following the experiment, we investigate wires with two different periods of modulation, Fig. 1(a) which has eight ''fingers,'' and Fig. 1(b) which has three ''fingers.'' The length of the wires is denoted by L and the width of the wide regions by W. Our calculations are performed on wires of the same size

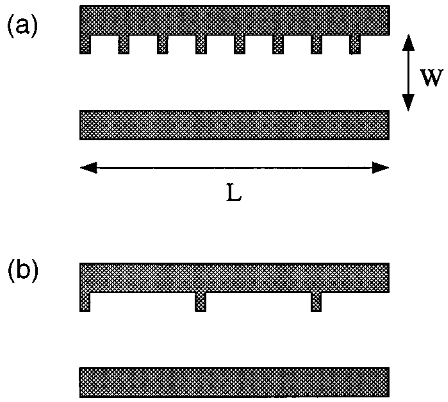

FIG. 1. Model geometries for quantum wires with two different periods of corrugation; eight fingers (a) and three fingers (b). The length and width are denoted by L and W.

as the experiment (lithographic gate size), $L=3$ μm and $W=1$ μm, as well as on narrower wires of width $W=5$ μm. The size of the fingers that periodically modulate the wire width is 0.1×0.2 μm.[2] The distance between the fingers is 0.3 μm in the eight-finger case, and 1.1 μm in the three-finger case. Our chosen Fermi energy (see below) corresponds to the number of propagating modes being $N=47$ in the wide wire, in the case of no corrugation. This number is close to the estimated number of modes in the experimental situation, which is roughly $N\approx 50$. We therefore expect our model parameters to well match the experimental system.

The model geometry is discretized on a 2D square lattice, where the lattice constant is chosen as $a=7$ nm. The wide wire geometry is hence 420×140 sites. Energies are conveniently measured in units of the tight-binding energy $|V| = \hbar^2/2\ m^* a^2$, which here is of the order of 10 meV. If the lattice constant is much smaller than the Fermi wavelength, $\lambda_F/a \gg 1$, we are in the parabolic part of the energy band, and the lattice model is assumed to give a good description of the true continuum system. We have chosen the Fermi energy to be $E_F=|V|$, which corresponds to the ratio $\lambda_F/a = 6.3$. Our model is thus expected to describe a continuum system quite well. The value of the Fermi energy in ''real'' units is $E_F=10$ meV and corresponds to a carrier density $n = 3.25\times 10^{15}$ m^{-2}. This value is very close to the experimental carrier density of Ochiai *et al.*,[14] $n=4\times 10^{15}$ m^{-2}.

The calculations are carried out using the recursive single-particle Green's-function technique. For a detailed description of the method we refer to previously published works.[17–21] Relations between the Green's functions and the **S** matrix of the system are employed,[22] which allow the conductance to be calculated from the generalized multichannel Landauer formula. The presence of a magnetic field, perpendicular to the plane of the constriction, is incorporated by means of a Peierls's phase factor. All calculations are performed at zero temperature. Therefore, we will get larger resistance fluctuations than in the experiment of Ochiai *et al.*,[14] which is performed at 0.65 K. This issue will be discussed further in the next section. When introducing random disorder in the system, we let each site energy vary randomly (with a uniform distribution) within an energy interval $\pm u/2$, where u is the disorder strength. This corresponds to the traditional Anderson disorder model. The lateral confining potential of the quantum wire is introduced by letting the site energy be very large in regions inaccessible to the electrons, i.e., hard-wall boundary conditions. To ensure numerical reliability of our computational scheme, we require that current conservation holds to a tolerance of 1×10^{-6}.

III. RESULTS AND DISCUSSION

In the following we present the calculated magnetoresistance for some different wire geometries. Even though the wires in the experimental setup of Ochiai *et al.*[14] are quasiballistic, we believe it is interesting also to study the influence of disorder. Diffusive systems, where the disorder is strong, have been widely investigated within the context of weak localization. It is interesting to study the interplay between the geometry-induced scattering and the random impurity scattering. A successive increase of disorder strength will take the system from the ballistic to the diffusive transport regime.[23] We will therefore vary the disorder strength, so for each geometry we calculate a set of plots, each plot corresponding to a different value of the disorder parameter. As expected, we find that for sufficiently strong disorder the weak localization effect disappears. This happens when the system approaches the diffusive regime, and impurity scattering dominates over the geometry-induced backscattering.

As mentioned above, the impurity scattering is introduced using the traditional Anderson model with on-site disorder, which is a convenient method for discretized geometries, and widely used to model diffusive and localized systems. For quasiballistic systems its suitability can be questioned, and this issue has been investigated.[24] However, we believe that for the type of qualitative understanding we are interested in here, the on-site disorder model will be of sufficient validity.

It is useful to relate the disorder parameter u to the elastic scattering length ℓ. In a 2D system, we have

$$\ell = \frac{6\lambda_F^3}{\pi^3 a^2}\left(\frac{E_F}{u}\right)^2. \qquad (1)$$

Throughout our calculations we will use the disorder parameter values $u=0$, 0.2, 0.3, and 0.5. The case $u=0$ corresponds to a purely ballistic situation, while the other cases correspond to the elastic scattering lengths $\ell=8$, 4, and 1 μm. When the elastic scattering length is larger than the wire length L, we will refer to this as the quasiballistic case ($\ell=8$ and 4 μm), while the parameter $\ell=1$ μm corresponds to entering the diffusive transport regime.

We start by calculating the magnetoresistance for the wide wire, $W=1$ μm, which is the lithographic size of the system of Ochiai *et al.*[14] The number of propagating modes is then $N=47$. In Fig. 2(a), the results for the eight-finger case are shown for different elastic scattering lengths. It is clearly seen that in the ballistic and quasiballistic regimes (three lower curves) the magnetoresistance has a negative slope, persisting up to approximately $B=0.1$ T. In the diffusive regime (top curve), no negative magnetoresistance can be seen. In the other cases, the negative magnetoresistance peak persists to much higher field strengths than in single quantum dots. In typical weak localization

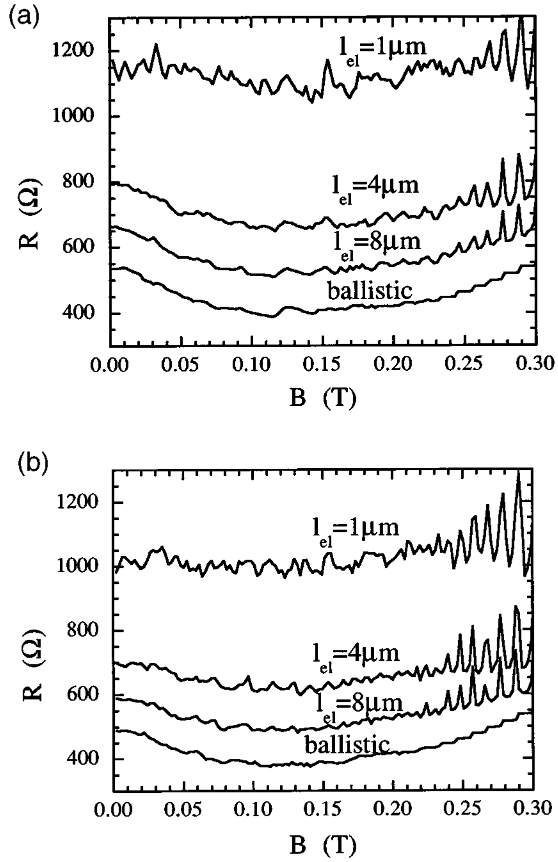

FIG. 2. Magnetoresistance for wire of width $W=1$ μm, for different elastic scattering lengths. (a) shows the eight-finger case and (b) shows the three-finger case. In the ballistic and quasiballistic regimes (three lower curves) the magnetoresistance has a negative slope, persisting approximately up to $B=0.1$ T. In the diffusive regime (top curve), no negative magnetoresistance can be seen. For higher B fields, edge-state effects occur. No significant dependence on corrugation period can be seen.

measurements,[8–11] the width of the peak is of the order of 1 mT, which is two orders of magnitude smaller than our value.

We interpret the surprisingly wide peak as a weak localization effect, arising from multiple backscattering and resonances among the segments of the corrugated wire. The periodically modulated width of the wire enhances backscattering, and therefore a stronger magnetic field is required to reduce self-trapping, which is the mechanism behind the weak localization effect. When the disorder parameter becomes so large that the system approaches the diffusive regime, random impurity scattering dominates over the periodic width modulation, and no negative magnetoresistance can be seen. As expected, the resistance fluctuations are also larger in this case.

For higher B fields, two types of phenomena occur in Fig. 2(a). One is the increase of the resistance, a result of the well-known depopulation of magnetoelectric subbands caused by a magnetic field. Secondly, when the B field becomes sufficiently strong (in this case $\sim$0.25 T), backscattering due to the periodic corrugation of the wire width becomes totally suppressed. The suppression of backscattering by a magnetic field is a well-known general phenomenon occurring in many different systems.[1,25] Consequently, well-resolved conductance steps appear in the ballistic case [bottom curve of Fig. 2(a)], each step corresponding to a magnetoelectric subband being switched off. In the quasiballistic and diffusive regimes [three upper curves in Fig. 2(a)], large resistance fluctuations occur each time a subband is switched off. The reason is that a mode being close to switch-off has a very small longitudinal momentum, and is therefore extremely sensitive to backscattering. Even weak disorder therefore results in large resistance peaks. The same phenomenon can be observed in quantum point contact systems, where, on a conductance vs gate voltage plot, the beginning of each step is most sensitive to backscattering.

When the B field becomes so strong that the cyclotron diameter is much smaller than the wire width, Landau levels take over the role of the magnetoelectric subbands. The cyclotron radius can be expressed as

$$\frac{r_c}{a}=\frac{1}{2\pi}\,\frac{h}{eBa^2}. \tag{2}$$

Taking our value of the Fermi energy, $E_F=10$ meV, at $B=0.1$ T the cyclotron radius is $r_c\approx 0.9$ μm, and at $B=0.25$ T we have $r_c\approx 0.4$ μm. The width of our wire is 1 μm, and consequently conductance quantization in the ballistic case appears when the B field is such that closed orbits begin to form. This is the regime where the transport is mainly due to edge states, and backscattering is therefore strongly suppressed.

Next we investigate the three-finger geometry, keeping all other parameters the same as in Fig. 2(a). The result is shown in Fig. 2(b). Qualitatively we obtain the same features as in the eight-finger case. A wide negative magnetoresistance peak appears in the ballistic and quasiballistic regimes, while no distinct features can be seen in the diffusive regime. Naturally, the fluctuations increase with increasing disorder strength. The finding of a weak localization effect also in the three-finger geometry is in good agreement with the experimental results of Ochiai *et al.* These authors measured the weak localization peak in geometries with eight, five, and three fingers, and found no significant dependence on the corrugation period.

Now we turn our attention to a narrower wire, width $W=0.5$ μm. This corresponds to the number of propagating modes being $N=24$. Figure 3(a) shows the case with eight fingers, for the same elastic scattering lengths as in Fig. 2. In the ballistic and quasiballistic case we observe the same trends as in the wide wire. The magnetoresistance has a negative slope, and the width of the peak is approximately 0.1 T. In the diffusive case the wide peak is absent, just as in Fig. 2. Interestingly, however, we find a much narrower peak in its place, as expected in the case of ‘‘traditional’’ weak localization. The width of this peak is approximately 0.01 T, i.e., ten times smaller than in the ballistic and quasiballistic cases. We therefore assume that in the diffusive regime, for this particular case, weak localization due to impurity scattering actually takes place. It is very illustrative to observe the gradual crossover between the ballistic regime, where the corrugation results in a weak localization effect, and the diffusive regime where impurity scattering dominates over the corrugation and traditional weak localization occurs.

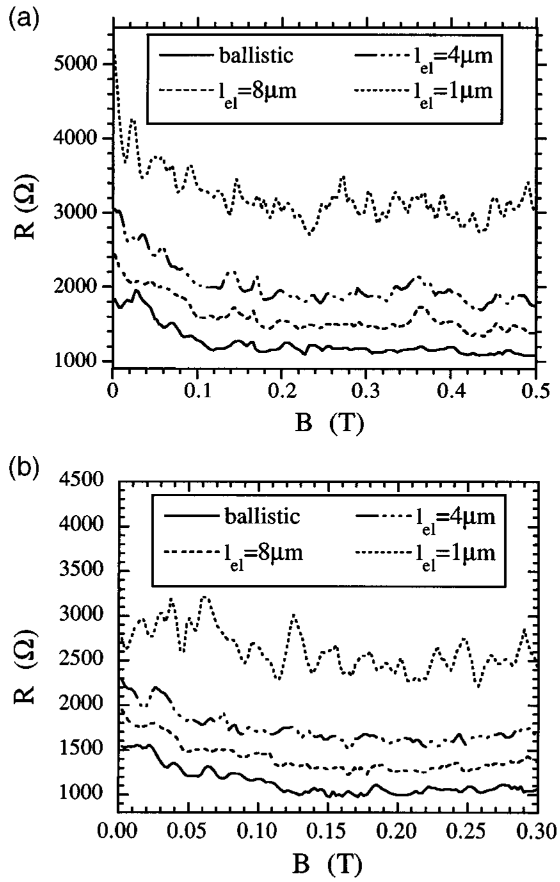

FIG. 3. Magnetoresistance for wire of width $W=0.5$ μm, for different elastic scattering lengths. (a) shows the eight-finger case and (b) shows the three-finger case. We find the same qualitative trends as in the wider wire of Fig. 2. The main difference is that in the diffusive case of (a), we observe a ''traditional'' weak localization peak, ten times narrower than the wide peaks.

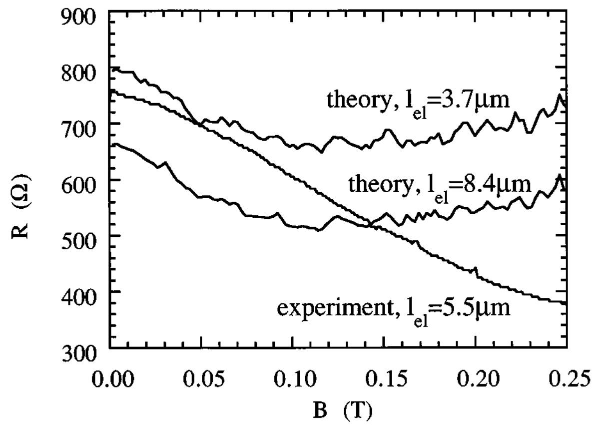

FIG. 4. Comparison between the calculated magnetoresistance (solid) and the experimental result (dotted) of Ochiai *et al.* (Ref. 14). The agreement is very good in the lower part of the *B*-field range. At strong *B* fields, the curves diverge. The experiment was performed at 0.65 K, while the calculations are done at zero temperature. Therefore, the experimental magnetoresistance is much smoother than the theoretical.

We wish to point out that we do not expect to see the traditional weak localization peak, in the diffusive regime, in all our wires. Each wire calculation is performed for one specific impurity configuration, i.e., only one ensemble member. Traditional weak localization, however, arises from taking an ensemble average over many different samples. When studying a single sample, one finds that it does not necessarily behave as the ensemble average, exhibiting the traditional weak localization peak. This issue has been discussed, and demonstrated experimentally.[26] Numerical simulations on ballistic cavities confirm these conclusions.[27]

For higher *B* fields we do not observe any edge state effects in Fig. 3(a). Since this wire is much narrower than that of Fig. 2, closed orbits do not form within the *B*-field range we are studying. Therefore, we cannot expect to find either magnetic depopulation, or conductance quantization, in this case.

In Fig. 3(b) we investigate the same type of wire as in Fig. 3(a), but with three fingers. Just as in the wider wire case, we do not find any significant dependence on corrugation period. In the ballistic and quasiballistic regimes a wide negative magnetoresistance peak is present, and as in the previous cases it disappears when entering the diffusive regime.

It is of interest to make a quantitative comparison between the experimental results of Ochiai *et al.*[14] and our numerical results. In Fig. 4 we plot the calculated magnetoresistance, in the quasiballistic case, for the eight-finger geometry, together with a corresponding experimental result of Ochiai *et al.*[14] The elastic scattering length in the experiment is approximately 5 μm, while our calculations are performed for the parameters $\ell=8$ and 4 μm. As can be seen in the figure, the agreement is very good in the lower *B*-field range. At higher *B* fields, where the resistance starts to increase due to the depopulation of subbands, the experimental and theoretical results begin to diverge. One reason for the disagreement could be that lattice effects enter in our model at strong *B* fields, and tend to overestimate the influence of the magnetic field.

We also need to keep in mind that the temperature is different in the theoretical and experimental case. Our calculations are done at zero temperature, while the temperature in the experiment is 0.65 K. The theoretical result therefore exhibits considerable resistance fluctuations, while the experimental curve is very smooth. The separation between energy levels is calculated to be 5 K at the Fermi level and 0.2 K between the two lowest-lying levels in our model. It is therefore reasonable to expect that the experimental temperature of 0.65 K will have a considerable smearing effect on the resistance fluctuations.

IV. DISCUSSION

We have calculated the magnetoresistance of quantum wires with periodically modulated width. The negative magnetoresistance peak was found to persist to much higher field strengths than in single quantum dots, the difference being roughly two orders of magnitude. Our results are in good agreement with some very recent experiments,[14] especially in the weak-field regime. The calculated negative magnetoresistance peak persists approximately up to 0.1 T. We believe that the wide peak is a manifestation of weak localization effect, arising from multiple backscattering and resonances among the segments of the corrugated wire. The weak localization effect is not sensitive to the period of corrugation, nor to the wire width, as long as the number of propagating modes is large.

The cause of the weak localization appears to be due to multiple backscattering from the corrugations themselves. Normally, weak localization arises from multiple backscattering from impurities (in the diffusive limit) and the interference between time-reversed paths, an effect which is broken up by a magnetic field of a few mT. Here, however, the effect persists to much higher values of the magnetic field, and is not due to the impurities within the corrugated wires. Beenakker and van Houten[1] suggest that such a long negative magnetoresistance can occur due to the reduction of backscattering from the entry point contact of the wire. However, this should also occur in single quantum dot structures, and this is not observed. While we cannot rule out such a possibility, it is more likely that the effect arises from multiple scattering within the wire, caused by the reflection of a small set of orbits from the protrusions themselves, and reflection of the electrons back into the entry contact. This will be much more difficult for the field to break up, since the field must deflect the particle completely around a protrusion as opposed to just deflecting it away from the time-reversed path of the diffusive transport. Such an interpretation is supported by the fact that the effect is eliminated in the strong scattering case, in which the onset of diffusive scattering of sufficient strength completely masks the role of the protrusions themselves.

When the impurity concentration is low, so that the elastic scattering length is larger than the wire length, the weak localization effect is not affected. However, when the elastic scattering length becomes smaller than the wire length, the negative magnetoresistance peak disappears. This happens when the random impurity scattering dominates over the geometry-induced scattering, as mentioned above. This tends to reinforce the interpretation that the weak localization here is due to the protrusions into the wire. For high B-field strength, in the edge-state regime, we observe a depopulation of subbands together with a suppression of backscattering. Clearly, magnetotransport properties in these geometries call for deeper investigations. In particular, a theoretical treatment of geometry-induced weak localization effect would be very interesting.

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[*]Present address: Ericsson Microwave Systems AB, S-431 84 Mölndal, Sweden.

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