Resonant reflection at magnetic barriers in quantum wires

Hengyi Xu and T. Heinzel

Condensed Matter Physics Laboratory, Heinrich-Heine-Universität, Universitätsstrasse 1, 40225 Düsseldorf, Germany

M. Evaldsson, S. Ihnatsenka, and I. V. Zozoulenko

Solid State Electronics, Department of Science and Technology, Linköping University, 60174 Norrköping, Sweden

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The conductance of a quantum wire containing a single magnetic barrier is studied numerically by means of the recursive Green’s function technique. For sufficiently strong and localized barriers, Fano-type reflection resonances are observed close to the pinch-off regime. They are attributed to a magnetoelectric vortex-type quasibound state inside the magnetic barrier that interferes with an extended mode outside. We, furthermore, show that disorder can substantially modify the residual conductance around the pinch-off regime.

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I. INTRODUCTION

Localized magnetic fields that are oriented perpendicular to a quantum film or a quantum wire, which are furthermore strongly localized in the transport (x) direction and homogeneous in the transverse (y) direction, are known as magnetic barriers (MBs). They can be realized experimentally by ferromagnetic films on top of a two-dimensional (or quasi-one-dimensional) electron gas residing in a semiconductor heterostructure: magnetizing the ferromagnetic film in the x direction results in a magnetic fringe field with a z component localized at the edge of the film that extends along the y direction. Transport experiments on MBs in two-dimensional electron gases show a pronounced positive magnetoresistance as a function of the MB amplitude, which can be interpreted quantitatively in a classical picture, where the MB acts as a filter with a transmission probability that depends on the angle of incidence of the electrons. Moreover, Peeters and Matulis studied the energy spectrum and the transmission properties of MBs with a rectangular profile in a two-dimensional electron gas by analytical means. This calculation predicts resonant structures in the low-energy region due to the presence of a virtual level.

MBs in quantum wires have been the subject of several theoretical studies recently, which are driven by the MB’s potential ability of parametric spin filtering, provided the effective g factor is sufficiently large. MBs are thus not only of fundamental interest but also have a distinct potential for application in spintronics. In these numerical studies, resonant features in the conductance are frequently found, e.g., in Fig. 3 of Ref. 10, Fig. 2 of Ref. 11, or Fig. 5 of Ref. 19. The character of these resonances as well as their origin have not been studied in detail. This, however, is not only of fundamental interest but also a prerequisite for possible applications. For example, the predicted spin polarizations can reach particularly high values in the proximity of such resonances.

Here, we use the recursive Green’s function technique to investigate the structure and the conductance of a single MB that forms in a quantum wire (QWR) below the edge of a ferromagnetic film. The barrier shapes are adapted from typical experimental conditions. We find that for smooth barriers with a large spatial extension, the number of transmitted modes drops stepwise and without resonances as the barrier amplitude increases or, correspondingly, the Fermi energy is reduced. As the lowest mode gets reflected, the conductance of weak barriers approaches zero as a function of decreasing energy, a situation that we denote as magnetic pinch-off. For sufficiently sharp barriers, however, pronounced dips in the conductance are found close to the pinch-off regime. From studies of the local density of states (LDOS) in combination with the spatially resolved occupation probability densities and current-density distributions, we conclude that the transmission zeros originate from the interference of an extended state with a quasibound vortex state that is localized inside the MB. This leads to resonant reflection and can be regarded as a type of Fano resonance. Furthermore, we discuss the influence of disorder on the reflection resonances.

II. MODEL AND CALCULATION METHOD

Let us consider a hard-wall QWR of length $L=4 \, \mu m$ in the x direction and width $W=500 \, nm$ in the y direction, defined in a semiconductor heterostructure with a ferromagnetic film placed on its surface (Fig. 1). We use the parameters of GaAs, i.e., an effective electron mass of $m_e=0.067m_0$ in our model, where $m_0$ denotes the mass of the free electron.

The ferromagnetic film has an in-plane magnetization $\mu_0M$ in the x direction, which generates a symmetric MB...
FIG. 2. The calculated conductance as a function of the Fermi energy $E_F$ for MBs of different localizations (distances of the QWR from the sample surface, calculated for a magnetization of $\mu_0M = 1.2$ T) and as a function of the barrier amplitude for $E_F = 25$ meV (upper inset). The lower inset shows the shapes of the MBs present at the distances considered, for the film magnetization assumed in the main figure. Here, $E_F = 22.5$ $\mu$eV denotes the ground-state energy.

$B_z(x)$. In-plane magnetic fields are neglected. The inhomogeneous MB can be expressed as

$$B_z(x) = -\frac{\mu_0 M}{4\pi} \ln \frac{x^2 + d^2}{x^2 + (d + h)^2}, \quad (1)$$

with $h$ being the thickness of the ferromagnetic film and $d$ the distance of the QWR from the semiconductor surface, respectively. As $d$ increases [which can be realized experimentally by preparing samples with two-dimensional electron gases at different locations in the growth (z) direction], the localization of $B_z(x)$ is reduced. A magnetization of $\mu_0M = 1.2$ T is assumed, which can be achieved experimentally by using Co$^{15}$ or Dy$^{18}$ as ferromagnetic material. It can be tuned by applying an external magnetic field in the x direction.$^{12,17}$ The Fermi energy can be adjusted by, e.g., a homogeneous gate electrode in between the semiconductor surface and the ferromagnetic film. We consider distances of $d = 15, 35$, and $350$ nm, which result in barriers of amplitudes $B_z(x=0) = 0.41, 0.28$, and $0.03$ T and full widths at half maximum (FWHM) of $94, 148$, and $812$ nm, respectively (see the lower inset in Fig. 2). Note that the integrated magnetic field $A = \int B_z(x) dx = 6.86 \times 10^{-8}$ Tm is independent of $d$.

The electronic wave functions in the quantum wire exposed to the MB structure $B_z(x)$ are described by the effective-mass Hamiltonian

$$H = H_0 + V_c(y), \quad (2)$$

where $V_c(y)$ is the confining potential in the transverse direction, which is assumed to be a hard-wall potential, and $H_0$ is the kinetic-energy term. Using the Landau gauge, the MB can be included by choosing the magnetic vector potential as $A = (-B_z(x)y, 0, 0)$. The kinetic energy can therefore be written as

$$H_0 = -\frac{\hbar^2}{2m} \left[ \left( \frac{\partial}{\partial x} - \frac{ieB_z(x)y}{\hbar} \right)^2 + \frac{\partial^2}{\partial y^2} \right]. \quad (3)$$

In order to perform numerical computations, the computational area is discretized into a grid lattice with lattice constant $a = 5$ nm, as shown in Fig. 1, such that the continuous values $x$ and $y$ are denoted by discrete variables $ma$ and $na$, respectively. Then the calculation area is connected to two ideal semi-infinite leads. The tight-binding Hamiltonian of the system reads

$$H = \sum_{m} \left\{ \sum_{n} \epsilon_0 c_{m,n}^\dagger c_{m,n} - t_c(c_{m,n-1}^\dagger c_{m,n} + e^{-i\phi_d} c_{m,n+1}^\dagger c_{m,n}) + H.c. \right\}, \quad (4)$$

where $\epsilon_0$ is the site energy which has included the effects of the bottom of the band and the confining potential, the hopping element $t_c = h^2/(2m^*a^2)$, and $c_{m,n}^\dagger$ and $c_{m,n}$ denote the creation and annihilation operators at the site $(m,n)$. The phase factor with $\phi_d = \frac{\pi}{2} \int_{x'} B_z(x') dx'$ is obtained by using the Peierls substitution.

In the presence of disorder, the site energy changes within a width $\Delta$, namely,

$$\epsilon_0 \rightarrow \epsilon_0 + \delta \epsilon_0, \quad (5)$$

where the values of $\delta \epsilon_0$ are distributed uniformly between $-\Delta/2$ and $\Delta/2$, and $\Delta$ is related to the elastic mean free path $\Lambda$ by

$$\Delta \over E_F = \left( \frac{6 \lambda_F}{\pi^2 a^2 \Lambda} \right)^{1/2}, \quad (6)$$

with $E_F$ being the Fermi energy and $\lambda_F$ the Fermi wavelength.

The two-terminal conductance $G_{21}$ is calculated within the framework of the Landauer-Büttiker formalism and can be expressed as follows:

$$G_{21} = \frac{2e^2}{h} \sum_{\alpha=1}^{N} |t_{\beta \alpha}|^2, \quad (7)$$

where $N$ is the number of propagating states in the leads and $t_{\beta \alpha}$ is the transmission amplitude from incoming state $\alpha$ in the left lead to outgoing state $\beta$. The transmission amplitudes $t_{\beta \alpha}$ can be expressed via the total Green’s function $G$ of the system as $t_{\beta \alpha} = \sqrt{\nu_{\alpha \beta}} G_{M+1,0}^{M+1,0}$, where $G_{M+1,0}^{M+1,0}$ denotes the matrix $\langle M+1 | G | 0 \rangle$, with $0$ and $M + 1$ corresponding to the positions of the left and right leads. We calculate $G_{M+1,0}$ on the basis of the recursive Green’s function technique in the hybrid energy space formulation.$^{27,28}$ We calculate separately the surface Green’s functions related to the left and right leads and the Green’s function of the scattering region with the MB, and then link them together at the boundaries. The wave function $\psi_i$ for the $i$th slice of the region under consideration is calculated recursively via

$$-\psi_i = G^{00} V^{i0} \psi_{0} + G^{ii} V^{i+1} \psi_{i+1}, \quad (8)$$

with $V$ the hopping matrix, and $G^{00}$ and $G^{ii}$ the shorthand notations of the Green’s functions $\langle 0 | G | 0 \rangle$ and $\langle i | G | i \rangle$. For visualization purposes, the current density $j_{nm}$ is associated with hopping along bonds and can be expressed as
we show equals zero within numerical accuracy. In the main figure, the conductance between the plateau at 2 with a maximum conductance up to magnetic pinch-off, the conductance shows a pronounced peak. In all our calculations, the electron temperature is set.

The local density of states at the site \( r = (m, n) \) is related to the total Green’s function in real space representation by the following equation:

\[
\rho(r; E) = -\frac{1}{\pi} \text{Im}[G(r, r; E)],
\]

where \( \text{Im} \) means the imaginary part of the complex matrix.

With this formalism, we study below a QWR with a hard-wall confinement potential and a maximum of four occupied modes outside the MB. We set the effective wall confinement potential and a maximum of four occupied modes.

III. RESULTS AND INTERPRETATION

In Fig. 2, the numerical results for ballistic QWRs are summarized. In the upper inset, the conductance of a QWR with two occupied modes is shown as a function of the barrier amplitude \( \mu_0 M \), for distances \( d \) of 15 and 35 nm, respectively. Quantized conductance steps are observed, which originate from reflections of the wire modes at the barrier and can be regarded in close analogy to the conductance quantization in quantum point contacts.29,30 Above the magnetic pinch-off, the conductance shows a pronounced peak with a maximum conductance up to \( =0.1 e^2/h \). We note that the conductance between the plateau at \( 2e^2/h \) and the peak equals zero within numerical accuracy. In the main figure, we show \( G \) as a function of \( E_F \) for the barriers given in the inset. For broad barriers, no structures close to the pinch-off regime are observed. As the localization of the MB or the number of occupied modes is increased, the number of conductance zeros increases as well. Here, however, we focus on the simplest scenario where just one resonance is present. This is the reason why we study QWRs with at most four occupied modes.

To shed some light on the origin of the structures in the conductance, we study the LDOS, integrated along the \( y \) direction, as a function of \( x \) (Fig. 3). For smooth MBs [Fig. 3(a)], the MB generates an \( x \)-dependent diamagnetic shift of the QWR modes, which are connected throughout the barrier structure. As the Fermi energy is lowered, barriers are formed for modes with subsequently lower energy, and again a stepwise decrease of \( G \) without resonances results.

As the barrier is localized further [Fig. 3(b)], the modes segregate and localized states form at the center of the barrier, which can be regarded as remnants of the magnetoelectric subbands. Qualitatively, we can understand this as follows. In sufficiently strong magnetic-field gradients, the magnetic phase changes abruptly in the \( x \) direction and pronounced reflections occur which localize the mode inside the barrier. These localized states may align in energy with the QWR modes of a higher index and a resonant reflection scenario results. The formation of localized states at the center of the MB is similar to the case of the double-barrier resonant tunneling (DBRT) structures, where transmission resonances are related to the existence of the quasibound states between two barriers. However, the present mechanism has a different phenomenology than DBRT: (i) in DBRT, the resonance transmission probability equals 1 for a symmetric structure. In our system, the transmission peak is much smaller than 1. (ii) DBRT structures do not possess transmission zeros. In our system, however, the dip in the conductance between the transmission peak and the first plateau equals zero within numerical accuracy. As the strength of the magnetic barrier increases, the height of the peak increases, but the transmission minimum remains at zero. (iii) For DBRT, the transmission resonances coincide with the quasibound states in energy and correspond to the poles in the complex-energy plane. However, in the present case, as can be observed in Fig. 3(b) (energy \( B \)), the maximum in the LDOS is at a different energy than the conductance peak. Rather, the peak position is at the low-energy tail of the
bound state. This phenomenology is the same as that found in waveguides with resonators attached.\textsuperscript{20-22} Following the discussion of Shao et al.,\textsuperscript{20} the resonator contributes a phase factor $\lambda$ and the transmission amplitude from left to right can be expressed as
\begin{equation}
\tau_{sl} = \tau_{d,sl} + \tau_{r,sl}(\lambda - r),
\end{equation}
with the transmission amplitudes $\tau_{d}$ and $\tau_{r}$ for being scattered into (from the left) and out (to the right) of the resonator, $r$, the factor of each reflection back into the resonator, and $\tau_{d,sl}$ the direct transmission path without a detour into the resonator. According to Eq. (11), the transmission amplitude can vanish if both a direct and an indirect transmission channel via the resonator are present and interfere with each other. This behavior corresponds to a Fano resonance,\textsuperscript{23} which is also found in systems related to ours.\textsuperscript{24,31,32}

In the following, we argue that this scenario does exist in a magnetic barrier under certain circumstances. The direct transmission channel is formed by an extended state which resembles an edge state in the region of high magnetic fields, while the bound state is a vortex state that forms near the center of the magnetic barrier. The character of such states is thus markedly different from snake-orbit states known from magnetic-field steps with a change in polarity.\textsuperscript{33}

To further illustrate this effect, we have studied the spatially resolved probability density and the current-density distribution emerging from the two occupied wave functions at the Fermi level close to the reflection resonance (see Fig. 4), where the sum of the probability densities $|\Psi_1|^2 + |\Psi_2|^2$ of the two wave functions (belonging to the first and second energy levels of the quantum wire) as well as the corresponding current-density distributions are plotted as a function of the lateral coordinates $x$ and $y$ for energies $A-D$. In the pinch-off regime at energies below the transmission resonance (for example, at energy $6.4E_1$, energy $A$), the region of high probability density inside the barrier is well separated in space from those in the leads. In addition, the probability of finding the electrons close to the barrier maximum is small. Correspondingly, the current density gets reflected at the flank of the barrier. As the energy is increased into the transmission peak (energy $B$), the region of high probability density moves along the $x$ direction into the barrier and a significant probability density is found even at the barrier maximum. At the same time, the probability density remains asymmetric about the center of the QWR in the $y$ direction. Translated into a current-density distribution, this means that inside the transmission peak, a current path evolves where the electrons enter the barrier region at the upper edge of the QWR, and while a large part of the electrons gets rejected, a significant fraction is transmitted, via the lower half of the QWR, to the right-hand side. At the reflection resonance (energy $C$), the region of high probability density is pushed even further into the barrier region, but, at the same time, develops a strongly symmetric shape about the center of the QWR cross section. This means that all the current flowing into the barrier gets reflected back into the QWR. At higher energies, the open regime is reached, like at energy $D$. It can be distinguished from the closed regime by the fact that a high probability density inside the barrier remains at only one edge of the QWR, which, at the same time, extends across the whole barrier structure in the $x$ direction. This structure provides a strong transmission channel for the electrons, with the current flowing predominantly at the lower right edge across the magnetic barrier. This behavior is a consequence of the formation of a local edge state inside the magnetic barrier.

Based on these findings, we interpret the resonances in the conductance as follows: close to the pinch-off regime, i.e., around $8E_1$ for $d=35$ nm in our model calculations, there is still a small but nonvanishing direct transmission probability through the magnetic barrier. This can be inferred from comparing the width of the transition region between the conductance plateaus 1 and 2, which is roughly $2.5E_1$ (see Fig. 2). The corresponding extended state has the character of an edge state in the magnetic barrier. According to Eq. (11), it interferes with the indirect transmission amplitude via the vortex-type bound state present in the magnetic barrier and generates a reflection resonance.

We proceed by discussing the effects of disorder on the transmission properties. In Fig. 5, the conductance around

![FIG. 4. Left column: grayscale plots of the sum of the probability densities $|\Psi_1|^2 + |\Psi_2|^2$ of the two occupied modes at the Fermi energy in the barrier region, shown for the energies marked in Fig. 2(b). The maximum of the MB is denoted by the dashed vertical lines, and its FWHM is 148 nm. Right column: the corresponding current-density distributions.](image)
FIG. 5. Conductance across the magnetic barrier around the reflection resonance for various degrees of disorder $\Delta/E_F$. The magnetization of the ferromagnetic film is $\mu_0 M = 1.2$ T, and the distance $d$ of the QWR from the surface is 35 nm. Note that the parameters without disorder are identical to those in Fig. 2.

...the reflection resonance is shown on a logarithmic scale as a function of the energy for various degrees of disorder. The disorder potential is modeled by a disorder $\Delta$ of the site energy. A critical disorder energy of $\Delta = E_F$ is observed. For lower disorder, the reflection resonance remains basically unaffected. At larger values for the disorder energy, the transmission at the resonance becomes nonzero, while the minimum in the conductance shifts toward larger energies. At $\Delta/E_F \approx 10$, the reflection resonance is no longer a characteristic property of the structure, while further resonances are of comparable strength. These resonances have their origin in interferences due to multiple reflections between impurities. We emphasize that while the specific disorder configuration taking the spin explicitly into account, it becomes clear that due to the resonance condition, particularly large spin polarizations can be expected around the resonances, the sign of which should be adjustable by a small change of the sample parameters. More studies are necessary to analyze the details of the spin effects in such resonances. Furthermore, we hope that our findings stimulate experimental studies with the objective of observing this type of reflection resonances.

IV. SUMMARY AND CONCLUSION

The conductance of quantum wires containing a magnetic barrier has been studied by the recursive Greens function technique. It is found that for sufficiently large ratios of $\mu_0 M/E_F$, the barrier “closes” and the transmission drops to zero. At energies close to the magnetic pinch-off, reflection resonances are observed for sufficiently localized magnetic barriers. The resonances have their origin in an interference between quasibound states residing inside the magnetic barrier and propagating states of the QWR which, at the magnetic barrier, have the character of edge states. Even without taking the spin explicitly into account, it becomes clear that due to the resonance condition, particularly large spin polarizations can be expected around the resonances, the sign of which should be adjustable by a small change of the sample parameters. More studies are necessary to analyze the details of the spin effects in such resonances. Furthermore, we hope that our findings stimulate experimental studies with the objective of observing this type of reflection resonances.

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*Electronic address: thomas.heinzel@uni-duesseldorf.de


