Resonant reflection at magnetic barriers in quantum wires

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The conductance of a quantum wire containing a single magnetic barrier is studied numerically by means of the recursive Greens 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 [1, 2] or a quantum wire [3, 4, 5, 6, 7, 8, 9, 10, 11], which are furthermore strongly localized in 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 [12, 13, 14, 15, 16, 17, 18] or quasi one-dimensional electron gas residing in a semiconductor heterostructure: magnetizing the ferromagnetic film in 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 [14, 15, 16, 17, 18], which can be interpreted quantitatively in a classical picture [15, 18], where the MB acts as a filter with a transmission probability that depends upon the angle of incidence of the electrons. Moreover, Peeters et al. [1] 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 [2].

MBs in quantum wires have been the subject of several theoretical studies recently, which is driven by their potential ability of parametric spin filtering [7, 8, 9, 10, 11], 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 has 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 [11].

Here, we use the recursive Greens function (RGF) 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 [12, 13, 14, 15, 16, 17, 18]. 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 zeroes originate from the interference of an extended state with a quasi-bound vortex state that is localized inside the MB. This leads to resonant reflection [20, 21, 22] and can be regarded as a type of Fano resonance [23, 24]. 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 x-direction and width \( w = 500 \text{ nm} \) in 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 \( m^* = 0.067 m_e \) in our model, where \( m_e \) denotes the mass of the free electron.
FIG. 1: Schematic representation of the considered two-terminal device, consisting of a MB created by a ferromagnetic film deposited on the top of a quantum wire. Also sketched is the square grid (period $a = 5 \text{ nm}$) used in the computation.

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 $\mu_0 M = 1.2 \text{ T}$), and as a function of the barrier amplitude for $E_F = 25 \text{ meV}$ (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, $E_1 = 22.5 \mu\text{eV}$ denotes the ground state energy.

The ferromagnetic film has an in-plane magnetization $\mu_0 M$ in $x$-direction, which generates a symmetric MB $B_z(x)$. In-plane magnetic fields are neglected. The inhomogeneous MB can be expressed as \[ B_z(x) = -\frac{\mu_0 M}{4\pi} \ln \frac{x^2 + d^2}{x^2 + (d + h)^2} \] (1)

with $h$ being the thickness of 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 $\mu_0 M = 1.2 \text{ T}$ 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 $x$-direction [12, 13, 14, 15, 16, 17]. The Fermi energy can be adjusted by, e.g., a homogenous gate electrode in between the semiconductor surface and the ferromagnetic film.

We consider distances of $d = 15 \text{ nm}$, $35 \text{ nm}$, and $350 \text{ nm}$, which result in barriers of amplitudes $B_z(x = 0) = 0.41 \text{ T}, 0.28 \text{ T}, 0.03 \text{ T}$, and full widths at half maximum (FWHM) of $94 \text{ nm}, 148 \text{ nm},$ and $812 \text{ nm}$, respectively, see the lower inset in Fig. 2. Note that the integrated magnetic field $A = \int B_z(x)dx = 6.86 \times 10^{-5} \text{ Tm}$ is independent of $d$.

FIG. 3: The local density of states (LDOS) integrated over the $y$-direction, as a function of energy and $x$. (a) For $d = 350 \text{ nm}$, the modes of the QWR experience a smooth diamagnetic shift in the barrier region, due to the formation of magnetoelectric subbands with spatially varying energy. (b) The LDOS for a strongly localized MB ($d = 35 \text{ nm}$) shows that the smooth evolution of the subband energies gets interrupted in the barrier region, and localized states form around the center of the barrier. Also shown is the position of the localized state in relation to the conductance of the structure.
The electronic wave functions in the quantum wire exposed to the MB structure $B_z(x)$ are described by the effective-mass Hamiltonian

$$H = H_0 + V_c(y)$$

(2)

where $V_c(y)$ is the confining potential in 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 magnetic vector potential as $A = (−B_z(x)y, 0, 0)$. The kinetic energy can therefore be written as

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

(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 $x, y$ are denoted by discrete variables $ma, na$, respectively. Then the calculation area is connected to two ideal semi-infinite leads. The tight-binding Hamiltonian of the system reads

$$H = \sum_m \left\{ \sum_n \epsilon_0 c_{m,n}^\dagger c_{m,n} - t \{ c_{m,n}^\dagger c_{m,n+1} + e^{-iqw} c_{m,n}^\dagger c_{m+1,n} + H.c. \} \right\}$$

(4)

where $\epsilon_0$ is the site energy which has included the effects of bottom of the band and confining potential, the
hopping element $t = \hbar^2/(2m^*a^2)$; $c^\dagger_{m,n}$ and $c_{m,n}$ denote
the creation and annihilation operators at the site $(m,n)$. The phase factor with $q = \frac{\pi}{L} \int_{x_{i+1}} B_z(x')dx'$ 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 $23$
$$
\frac{\Delta}{E_F} = \frac{6\lambda_F^3}{\pi^2 a^2 \Lambda^{1/2}} \quad (6)
$$
with $E_F$ being the Fermi energy and $\lambda_F$ the Fermi wavelength.

The two-terminal conductance $G_{2t}$ is calculated within the
framework of the Landauer-Büttiker formalism and can be expressed as following $29$
$$
G_{2t} = \frac{2e^2}{h} \sum_{\beta,\alpha=1}^{N} |t_{\beta\alpha}|^2 \quad (7)
$$

where $\psi_{mn}$ is the wave function at site $(m,n)$, and $\mathbf{m}, \mathbf{n}$
are the unit vectors in the longitudinal ($x$-) and transverse ($y$-) direction.

The local density of states at the site $\mathbf{r} = (m,n)$ is related to the total Green’s function in real space representation by the following equation $24$
$$
\rho(\mathbf{r}; E) = -\frac{1}{\pi} \text{Im}[G(\mathbf{r}, \mathbf{r}; E)] \quad (10)
$$
where 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 4 occupied modes outside the MB. We set the effective g-factor to zero, therefore the modes always have a spin degeneracy of 2. Via the distance $d$, the barrier itself is varied in both amplitude and localization (characterized by its FWHM) at fixed Fermi energy $E_F$. Alternatively, we vary $E_F$ and keep the MB constant. In all our calculations, the electron temperature is set to zero.

### 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 2 occupied modes is shown as a function of the barrier amplitude $\mu_0 M$, for distances $d$ of 15 nm 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 $23, 30$. Above the magnetic pinch-off, the conductance shows a pronounced peak with a maximum conductance up to $\approx 0.1 e^2/h$. 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 zeroes 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 local density of states (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 $x$-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 zeroes. 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 quasi-bound 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 wave guides with resonators attached [20]. Following Shao’s discussion, the resonator contributes a phase factor $\lambda$ and the transmission amplitude from left to right can be expressed as

$$t_{rl} = t_{d,rl} + t_{rs} t_{st} / (\lambda - r_s)$$

(11)

with the transmission amplitudes $t_{st}$ and $t_{rs}$ for being scattered into (from the left) and out (to the right) of the resonator and $r_s$ the factor from each reflection back into the resonator, and $t_{d,rl}$ denotes 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, which is also found in systems related to ours [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 [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 level 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 $6.4 \times E_1$, 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 $y$-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 $x$-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 non-vanishing 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 $2.5 \times E_1$ (see Fig. 2). The corresponding extended state has the character of an edge state in the magnetic barrier. According to Eq. (11), it interferes...
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 $\mu_0 M = 1.2 \, \text{T}$, 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.

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 the reflection resonance is shown on a logarithmic scale as a function of the energy for various degrees of disorder. The disorder potential is modelled by a disorder $\Delta$ of the site energy. A critical disorder energy of $\Delta \approx E_F$ 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 towards 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 at fixed $\Delta/E_F$ determines details of the energy-dependent conductance, it does only marginally influence the position, the minimum conductance or the width of the reflection resonance.

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 drop 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 quasi-bound 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 to observe this type of reflection resonances.

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