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Abstract

We present numerical simulations of the transport properties of a ballistic cavity connected to two leads in the presence of a finite degree of decoherence. The cavity is obtained by realizing a ‘quantum chicane’, i.e., by shifting a short section of a quantum wire defined by etching on a SiGe heterostructure. We compare our results with experiments by Scappucci \textit{et al} (2004 \textit{Trends in Nanotechnology} (Segovia, Spain, Sept. 2004) unpublished) and show that the magnetoconductance features can be reproduced if we use a recently developed model that includes decoherence with a phenomenological statistical description. Otherwise, simulations based on completely coherent transport would provide a much richer structure of magnetoconductance, that in experiments is smoothed out by dephasing processes. In particular, we recover experimental features of the magnetoconductance such as magnetic focusing and Shubnikov–de Haas oscillations. By computing the local partial density of states of the system at different values of the external field we recover the semiclassical orbits.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Mesoscopic devices such as ballistic cavities deal with physical phenomena governed both by quantum mechanical mechanisms, such as interference due to the phase coherent propagation of the wavefunction, and by semiclassical mechanisms, when a large number of conducting channels contribute to transport.

Weak localization (WL) originating from enhanced backscattering and Shubnikov–de Haas (SdH) oscillations of the magnetoconductance originating from magnetic quantization of energy levels belong to the first category [2, 3]. Magnetic focusing (MF) due to commensurability between the classical cyclotron orbit $r_c$ and the cavity length belongs to the latter [4–6]. Such conductance modulations are usually controlled by varying the carrier density through gate voltages or by varying the externally applied magnetic field.

In the ballistic transport regime, and when the temperature is of the order of few tens of mK, so that temperature smearing is negligible, other resonance phenomena such as multiple reflections in the cavity may occur, that lead to rapid and wide oscillations of the conductance when a gate voltage or the magnetic field are swept, so that other conductance modulations are not visible anymore.

Luckily, in experiments it often occurs that only magnetic focusing and SdH oscillations are observed, since they are more robust to the effects of decoherence due to interaction with the environment [4, 7, 8]. Therefore, from the simulation point of view, we can observe MF and SdH oscillations if we are able to introduce a finite degree of dephasing in the transport mechanism.

In this paper we present numerical simulations of magnetotransport in a ballistic cavity obtained by transversally shifting the central section of a quantum wire defined on an SiGe heterostructure and hence generating two constrictions.
behaving as quantum point contacts. Such a structure has been experimentally fabricated and characterized as described in [1, 9]. We obtain the 2D confining potential by computing the first subband profile from a self-consistent solution of the 3D Schrödinger–Poisson equation on the whole structure and compute the magnetoconductance and the local partial density of states with a code based on the computation of the scattering matrix of the system. The effect of dephasing on the transport properties is included with a statistical treatment of the dephasing process described in a recent work [10]. We are able to recover MF and SdH oscillations of the magnetoconductance curve, assuming negligible corrections to the potential due to the change of the external magnetic field. In this way, the computational resources required are still tractable.

We obtain the quantum conductance \( G \) at zero temperature using the Landauer–Büttiker formula [16, 17] that expresses \( G \) as a function of the transmission matrix \( T \). The conductance of a generic device depends on the transmission probability matrix \( T = tt^\dagger \) through the formula

\[
G = g \frac{e^2}{h} \sum_n T_n, \tag{4}
\]

where \( g \) is the degeneracy factor (\( g = 4 \) in our case due to both spin and valley degeneracy) and the sum is over the all the eigenvalues \( T_n \) of the transmission probability operator \( T \). The numerical method is based on the computation of the scattering matrix of the conductor. First, the domain is subdivided into several slices along the propagation direction. For each slice \( j \) one can easily compute the scattering matrix \( S_j \) by solving the 2D Schrödinger equation with Dirichlet boundary conditions on the transversal cross section and by enforcing continuity of the wavefunction and of the probability current density between adjacent slices. \( S_j \) has the form

\[
S_j = \begin{pmatrix} r_j & t'_j \\ t_j & r'_j \end{pmatrix}, \tag{5}
\]

where \( t_j \) (\( t'_j \)) and \( r_j \) (\( r'_j \)) are the transmission and reflection matrices, respectively, from left to right (right to left). In order to compute the total scattering matrix \( S_T \), it is sufficient to compose all the \( S_j \) matrices [3].

Finally, the presence of a magnetic field \( B = B\hat{z} \) perpendicular to the propagation plane \( xy \) is taken into account by adopting the transverse gauge \( A = Bx\hat{y} = A(x)\hat{y} \) for the vector potential \( A = \nabla \times B \). The new Hamiltonian can be written as the sum of two terms: \( H(\mathbf{x}, y) = H_{\text{trans}}(y) + H_{\text{long}}(x) \), where \( H_{\text{trans}} = [p_x - eA(x)]^2/2m_y + V(y) \) refers to the transversal part of the Hamiltonian and \( H_{\text{long}} = p_x^2/2m_x \) to the longitudinal one. The eigenvectors are given by the product of the eigenvectors for the two Hamiltonians, that are plane waves for \( H_{\text{long}} \) and

\[
\chi_{n,j}(y) = \chi_{n,j}^0(y) \exp[-ieA(x)/\hbar] \tag{6}
\]

for \( H_{\text{trans}} \), where \( \chi_{n,j}^0(x) \) are the solutions in the case \( B = 0 \). Furthermore, with this gauge, the eigenvalues \( E_{j,n} \) are not altered by the presence of the magnetic field. We note that the condition for the validity of the discretization of \( H_{\text{trans}} \) is that the magnetic flux through a generic slice \( |A(x,y) - A(x)| \) \( W \) is much smaller than the quantum unit of flux \( h/e \), where \( W \) is the transverse device length [18].

3. Dephasing model

In this section we briefly describe a phenomenological approach for including dephasing in the simulation of

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The scattering matrix technique is a powerful tool for describing the transport properties of mesoscopic systems, particularly in the context of quantum confinement. In this section, we will focus on the study of magnetoconductance in SiGe cavities, which are a type of mesoscopic device made from silicon and germanium.

**Mesoscopic Devices**

Mesoscopic devices, such as quantum wires and cavities, are systems where quantum effects become dominant due to their small size. The scattering matrix technique is particularly useful in these systems because it allows for the description of transport properties in terms of the scattering of particles at interfaces and within the device.

**The Scattering Matrix Technique**

The scattering matrix technique involves the use of a matrix $S$ that describes the propagation of particles through a quantum system. This matrix is defined as $S = T R$, where $T$ is the transmission matrix and $R$ is the reflection matrix. The reduced scattering matrix, $S_{j,j'}$, is obtained by averaging the conductance over a mesh size used varies from 0.5 to 2 nm along the longitudinal direction and a 2D electron gas is located in the strained-Si channel.

**Quantum Cavities**

Quantum cavities, such as those shown in Figure 1, are confined structures that can support a variety of modes. The magnetoconductance obtained by Scappucci et al. [1] at 50 mK three magnetic focusing oscillations with conductance peaks at $B = 0.1, 0.25$, and $0.43$ T, and minima for $B = 0.17$, and $0.33$ T. For higher magnetic field, SdH oscillations appear, whose frequency allows us to extract an mode in the $j$th slice. We modify each element by adding a random phase $\delta\phi$ so that the generic diagonal element of the transmission matrix is $e^{i\delta\phi_{jk}}$ and $\delta\phi$ is extracted by a random number generator and obeys a zero average Gaussian distribution with variance $\sigma^2 = d_j/4\hbar$. The total scattering matrix obtained in such a way only represents a particular occurrence of the reduced scattering matrix of the single particle. The average reduced scattering matrix is obtained by averaging the conductance over a sufficient number of runs, typically of the order of one hundred. In this way we take into account the intrinsic statistical character of the dephasing process. We emphasize that the usual properties of the scattering matrix $S$, such as unitarity $SS^\dagger = I$ and the Onsager–Casimir relations [22] for the reciprocity relations of the scattering matrix, still hold [10].

**4. Magnetoconductance of SiGe Cavities**

We now present results from our simulations of the considered cavity. The structure is depicted in figure 1 and consists of an SiGe heterostructure with the same layer structure described in [9]. Quantum confinement is present along the growth direction and a 2D electron gas is located in the strained-Si channel.

A quantum wire with a width of 250 nm is considered and a section of a length of 570 nm is laterally shifted in order to form a cavity separated from the leads by two quantum constrictions. The two constrictions have a geometrical width of 80 nm, and a much smaller electrical width, as shown in figure 2, where the lowest 2D subband for electrons near one constriction is shown, as obtained from the 3D Poisson–Schrödinger solver. The mesh size used varies from 0.5 to 2 nm along the longitudinal direction (x-axis) and is fixed to 2.5 nm along the y-axis.

The magnetoconductance obtained by Scappucci et al. [1] presents at 50 mK three magnetic focusing oscillations with conductance peaks at $B = 0.1, 0.25$, and $0.43$ T, and minima for $B = 0.17$, and $0.33$ T. For higher magnetic field, SdH oscillations appear, whose frequency allows us to extract an...
electron density of about $7 \times 10^{11}$ cm$^{-2}$. From such a value of the electron density we can infer that only one mode propagates through each constriction.

In figure 3 we show the magnetoconductance of the cavity for a Fermi energy of $E_F = 3$ meV, corresponding to only one propagating mode through the constriction. We plot the coherent case (solid curve, $l_0 \to \infty$), the case $l_0 = 5 \ \mu$m (dashed curve), and $l_0 = 1 \ \mu$m (dash–dotted curve). The partially coherent cases are obtained from a Monte Carlo simulation on an ensemble of 300 runs as described in section 3. Let us stress the fact that resonances due to multiple reflections in the cavity are destroyed by the effect of decoherence. Such resonances are not present in the coherent calculations at high magnetic field, when transport occurs through edge channels. The second effect of the decoherence is to reduce the amplitude of tunable resonances due to MF and SdH oscillations.

The first three maxima of the magnetoconductance are obtained for $B = 0.04$, 0.23, 0.43 T, minima appear for $B = 0.12$, 0.35 T. The agreement with the experiment is very good, also considering the fact that the geometry of the simulated structure only approximates the actual geometry.

Finally, in figure 4 we show the colour plot of the local partial density of states of the system for three specific values of the magnetic field corresponding to two MF peaks in the magnetoconductance plot (states injected from the left) and one minimum. The local density of states $\rho(x_i, y_j, E) = |\Psi(x_i, y_j, E)|^2$ is computed by calculating the wavefunction of the system at each point $(x_i, y_j)$ of the grid with a recursive scattering matrix method. It is interesting to verify that for $B = 0.23$ and 0.43 T we are able to appreciate the pattern of the semiclassical orbit. For $B = 0.23$ T we have $L \sim r_c$, and for $B = 0.43$ T we have $L \sim 2r_c$. For $B = 0.35$ T, corresponding to a conductance minimum, the local density of states reveals very complicate trajectories.

5. Conclusion

In this paper we have presented a numerical simulation of the transport properties of a strained Si–SiGe ballistic cavity. In particular we studied the effects of environmental dephasing in attenuating the oscillation amplitudes and in cancelling dense resonances due to multiple scattering inside the cavity.

We were able to destroy such uncontrolled resonances and to preserve magnetoconductance oscillations by choosing a degree of decoherence with a coherence length slightly larger than the structure length. Moreover, we presented simulations of the density of states of the system when the applied magnetic field is such that the cyclotron radius is commensurable with the size of the cavity or with a sub-multiple and recover patterns of semiclassical orbits, ensuring the semiclassical origin of such resonances.

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