Spin-dependent transport in double ferromagnetic-gate graphene structures

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Abstract. Based on the non-equilibrium Green’s function method recently developed to solve the quantum relativistic-like Dirac’s equation, spin dependent transport in double ferromagnetic-gate graphene structures has been investigated. The study is focused on the possibility of controlling the spin polarization and the tunnelling magneto-resistance by the gate voltages. Different from the case of ordinary semiconductors, obtained results show that the transport depends weakly on the well width, but strongly on the confined hole states in the gated regions.

Keyword: Spin polarized transport, Klein tunnelling, Green’s functions method, graphene.

1. Introduction
Graphene is a single layer of carbon atoms filling in a honeycomb lattice with the lattice constant of ~0.14 nm. This novel material was discovered in 2004 [1] and has been attracting a lot of attention, from both experimental and theoretical viewpoints, in different fields of research, e.g., condensed matter physics [2], materials science [3] and device applications [4]. This intensive interest is due to the unique electronic properties of graphene such as the gapless and the conical-shape of the electronic structure around the Dirac points (or the K-points). Accordingly, the low energy excited states behave as those of massless relativistic-like particles with the typical charge-conjugation symmetry between the electron and the hole states. These lead to observations of specific and anomalous transport phenomena in this single carbon-atomic layer, e.g. the finite value of the conductance at zero-concentration [3], the spin valve effect [5], the unusual half-integer quantum Hall effect [6], etc. Such phenomena can be successfully described using the massless fermion Dirac’s model [7].

Because of high mobility and gate-controllable carrier conduction, graphene appears to be very promising for designing high performance transistors. Additionally, due to very weak spin orbit interaction [8, 9] which leads to a long spin flip length (~1 μm) [5], it offers good potential for spintronics applications [10]. Some possibilities of inducing ferromagnetism in graphene have also been discussed. For instance, the ferromagnetism can be intrinsically induced in graphene by defects [11, 12], impurities [13] or by using an external electric field [14]. Haugen et al. [15] recently suggested that the ferromagnetic correlations can be externally induced in graphene by the proximity effect of a magnetic gated insulator deposited on the graphene sheet. Moreover, possibilities of...
controlling the spin current in single ferromagnetic-gate graphene structures have been discussed [16, 17]. However, such studies are usually based on the scattering matrix approach which is intuitive but difficult to implement in a general framework, for instance including some important effects as scattering by impurities and defects. Recently, we have developed a calculation method based on the nonequilibrium Green’s functions (NEGF) to solve the massless fermion Dirac’s equation [18]. The approach has been efficiently applied to study the electronic transport and the spin polarization effect in single gate graphene structures. In this work, we use that method to study the spin dependent transport in double ferromagnetic-gate graphene structures, as schematized in figure 1. Our study is focussed on the role of confined charge states in both the well and the gated regions and on the analysis of the two typical quantities, the spin polarization (P) and the tunnelling magnetoresistance (TMR).

2. Model and formulation
The considered double ferromagnetic-gate structure is modelled by the Dirac-like Hamiltonian

\[ H = v_f \left( \sigma_x p_x + \sigma_y p_y \right) + Q, \]

where \( v_f = 10^6 \text{m} \text{s}^{-1} \) is the Fermi velocity; \( \sigma_x \) and \( \sigma_y \) are the Pauli matrices; \( p_x \) and \( p_y \) are the momentum operators; and

\[ Q(x) = [U_1 - \eta \Delta] \Theta(x) \Theta(L_1 - x) + [U_2 + \eta \Delta] \Theta(x - L_1 - W) \Theta(L_1 + W + L_2 - x), \]

where \( \Theta \) is the Heaviside step function used to define the two gated regions. The potential barrier \( U_{1(2)} > 0 \) is tuned by the gate voltage \( V_{G1(G2)} \) all along the gate length \( L_{1(2)} \). The two gated regions separating the source/drain leads from the well are covered by a ferromagnetic insulator, which will induce the exchange splitting \( \Delta \) in graphene. \( \eta = \pm 1 \) stands for the spin orientation of conduction electrons in the structure. The magnetic moment of the gated region 1 is fixed while that of the gated region 2 may be reversed.

![Figure 1. Sketch of the potential along the considered double ferromagnetic-gate graphene structure.](image)

Within the model described by equation (1), the transport is considered to be ballistic according to the NEGF formalism. The transport quantities can be determined through the transmission coefficient which is expressed in terms of the retarded and advanced Green’s functions \( G^{r,a} \) as

\[ T(E) = \sum_{n,m}^2 \Gamma_{1,n} G_{n,2,n-1} \Gamma_{2,n} G_{2,n-2,m,1}, \]

where \( \Gamma_{1,n} = i \left( \Sigma^{r}_{n} - \Sigma^a_{n} \right) \) is defined in terms of the retarded and advanced self-energies \( \Sigma^{r,a} \) which describe the coupling between the graphene sheet and the source (drain) electrode. The conductance is then calculated using the Landauer formula [19]. Similar to Ref. [18], hereafter, the temperature is...
chosen to be zero for simplicity and the energy unit is \( E_0 = \hbar v_F / 2a \), where the mesh-spacing \( a \) is 0.2nm.

On the basis of the above formalism, the spin polarization \( P \) and the tunnelling magnetoresistance \( TMR \) are determined by

\[
P = \frac{G_\uparrow - G_\downarrow}{G_\uparrow + G_\downarrow},
\]

\[
TMR = \frac{G_P - G_{AP}}{G_P + G_{AP}},
\]

where \( G_{\uparrow(\downarrow)} \) corresponds to the conductance for up (down) spin channel and \( G_{P(\text{AP})} \) is the conductance for parallel (anti-parallel) alignment configuration of the magnetic moments.

3. Numerical results and discussions

As discussed in Ref. [18], due to the confined hole states inside the barrier (gated) regions, the conductance of each spin channel oscillates versus the barrier height. The exchange splitting, which shifts the conductance of the spin channel relatively to each other, can lead to the oscillation of the spin polarization \( P \) and of the \( TMR \) as well. We display in figure 2 the dependence of \( P \) and \( TMR \) on the barrier height \( U_1 \) while the barrier height \( U_2 \) is fixed in a symmetric structure with \( L_1 = L_2 = 20 \) nm. In this case, the spin polarization behaves similarly to that in the case of the single barrier (single gate) structures, i.e., it is an oscillatory function of \( U_1 \) or/and the exchange splitting \( \Delta \). But for appropriate values of \( \Delta \), the spin polarization \( P \) can be a positive/negative-definite function of the barrier height [e.g., \( \Delta = 0.015 \) or/and \( \Delta = 0.045 \)]. The period of the oscillation is then estimated to be \( U_P = \frac{2\pi a}{L_1} \). For instance, for \( L_1 = 20 \)nm the period is \( U_P \approx 0.062 \). When tuning \( \Delta \), this period does not change but the amplitude of the oscillations does.

![Figure 2](image_url)

**Figure 2.** (Colour online) Oscillations of the spin polarization and the correlated \( TMR \) as a function of the barrier height \( U_1 \) in a structure: \( L_1 = W = L_2 = 20 \) nm. The Fermi energy \( E_F \) in the source-drain leads and the well is 0.1. The figures (a) and (d) [(b) and (c)] correspond to the parallel (anti-parallel) alignment of the magnetic moments. In the left column: \( \Delta = 0.015 \) (solid), 0.03 (dashed) and 0.045 (solid-circle) with \( U_2 = 0.4 \). In the right column: \( U_2 = 0.34 \) (solid), 0.37 (dashed) and 0.4 (solid-circle) with \( \Delta = 0.015 \).
For the TMR, the period of the oscillation is about $\pi a / L_1$ which is one half of that of the spin polarization (see the left column of figure 2). This agrees well with the estimation in Ref. [15] where $TMR \approx P^2$ in symmetric structures. Moreover, the maximum (minimum) of the spin polarization $P$ for the parallel configuration corresponds to the minimum (maximum) of that for the anti-parallel one. Because the two barriers are equivalent, $P$ and TMR also oscillate when changing $U_2$ with the period $2 \pi a / L_2$ (see the right column of figure 2). However, the spin polarization is completely suppressed for the anti-parallel configuration if $L_1 = L_2$ and $U_1 = U_2$ when the pictures of the confined hole states are the same in the two barrier regions.

![Figure 3](Colour online) Oscillations of the spin polarization as a function of the barrier height $U_1$ in an asymmetric structure: $L_1 = W = 20$ nm, $L_2 = 30$ nm, $U_2 = 0.4$, $E_F = 0.1$ and for different values of $\Delta$: 0.02 (a), 0.03 (b) and 0.045 (c). The solid (solid-circle) curve corresponds to the parallel (anti-parallel) alignment. The correlated TMR (d) is also plotted for: $\Delta = 0.02$ (solid), 0.03 (dotted) and 0.045 (dashed).

To investigate the effect of asymmetry of the gate lengths, we present in figure 3 the obtained results for a structure with $L_1 = 20$ nm and $L_2 = 30$ nm. It is interesting to note that by tuning $\Delta$ one can find some values which satisfy the condition $\Delta = n\pi a / L_1$ or $m\pi a / L_2$ (e.g. $\Delta = 0.02$ or 0.03) for which the hole states in the gated region 1 or the gated region 2 are identical for the two spin channels. Hence the structure behaves similarly to the case of a ferromagnetic barrier coupled with a normal (nonmagnetic) barrier. This leads to identical spin polarization for the parallel and the anti-parallel configurations and therefore a complete suppression of the TMR. If the above condition is not satisfied, e.g., $\Delta = 0.045$, the spin polarizations for the parallel and for anti-parallel configurations are different and the TMR is an oscillatory function of the barrier height. Moreover, in this case, the spin polarization for the anti-parallel configurations does not vanish when $U_1 = U_2$.

Since the conductance does not only oscillate versus the barrier height, but also as a function of the exchange splitting, one can expect a modulation of these oscillations when changing another parameter such as the gate lengths [17, 18]. Indeed, figures 4 and 5 show the beating behaviour of the spin polarization and the TMR versus the gate length $L_1$ for different values of $\Delta$ and $U_2$. The period of this modulation can be estimated to be $L_p \approx 2\pi a / \Delta$ [for example, with $L_p \approx 61.5$ nm and $L_p \approx 30.6$ nm for $\Delta = 0.02$ and $\Delta = 0.04$, respectively, see figure 4]. For $\Delta = 0.03$ ($= \pi a / L_2$), as discussed above, the modulation effect of the spin polarization is also similar to that of the single ferromagnetic gate structure and the TMR is suppressed. In comparison with the results presented in figure 2, we additionally remark that when tuning $U_2$ (figure 5), the mean value and the amplitude of the spin polarization and TMR oscillate with the period $2\pi a / L_2$ but the phase of modulated oscillations seems to be unchanged.
Another point is the possible role of the well width $W$ (separating the two gates). It is well-known that in double barrier structures based on normal semiconductors, this layer is very important since states of charge are quantized and govern the transport properties of the system. However, for the structures under study here, the numerical results show that the conductance and also the spin current depend weakly on the width $W$. In contrast, the alignment of the confined hole states inside the two barrier regions is important, which is nothing, but the resonant transport condition.

4. Conclusion

We have studied the spin current in double ferromagnetic-gate graphene structures by using NEGF formalism. We find that, due to the exchange splitting in the gated regions, the spin polarization and TMR have an oscillatory behaviour with respect to the barrier heights, which can be tuned by the gate voltages, and exhibit modulating behaviour related to the gate lengths. The study also shows that not the confined charge states in the well, but the alignment of the hole states inside the gated regions,
responds for the resonant transport condition which leads to the oscillation of the spin current. The simulation technique developed and these results may provide an additional understanding of the spin dependent transport in graphene-based spintronic devices.

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