Spin-orbit interaction in chiral carbon nanotubes probed in pulsed magnetic fields

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The magnetoconductance of an open carbon nanotube (CNT)-quantum wire was measured in pulsed magnetic fields. At low temperatures, we find a peculiar split magnetoconductance peak close to the charge-neutrality point. Our analysis of the data reveals that this splitting is intimately connected to the spin-orbit interaction and the tube chirality. Band-structure calculations suggest that the current in the peak regions is highly spin polarized, which calls for application in future CNT-based spintronic devices.

An efficient source of spin-polarized electrons is one of the important building blocks of a future spin-based electronics.1 Very high degrees of polarization can potentially be achieved by exploiting spin-orbit interaction (SOI).2,3 Based on the low atomic number Z=6 of carbon, the spin-orbit interaction in carbon nanotubes (CNTs) was mostly believed to be very weak, until a recent experiment4 has demonstrated the effect of spin-orbit interaction in clean CNT quantum dots.

In this Rapid Communication, we present magnetoconductance (MC) data for the complementary situation of an open CNT-quantum wire obtained in pulsed magnetic fields. Open quantum wires allow much higher currents (up to microampere) since a whole band participates in the transport rather than the individual levels in the quantum-dot regime. In a parallel magnetic field $B_{||}$, a small band-gap CNT evolves via a metallic state into a semiconducting one, resulting in a typical peak in the MC.5,6 In one of our tubes, however, we observed a splitting of this MC peak into two peaks at low temperature. Recording MC traces at different gate voltage $V_g$, shows that the splitting vanishes when moving away from the charge-neutrality point (CNP). A thorough comparison to band-structure calculations reveals that the splitting is explained by the SOI, which becomes strong for small tube diameters. Our analysis predicts a highly spin-polarized current in the peak regions.

The experiments have been performed on devices made of individual CNTs prepared on Si/SiO$_2$/Si$_3$N$_4$ substrates. The heavily $p$-doped Si was used as a backgate and the thickness of the insulating layer was 350 nm. CNTs were grown by means of a chemical vapor deposition method7 and Pd (50 nm) electrodes were defined on top of the tubes by e-beam lithography. In order to exclude strain effects on the band structure,8 only straight and long ($\sim$50 $\mu$m) CNTs were selected for devices and the distance between two Pd electrodes was $\sim$500 nm. The dc magnetoconductance was studied in pulsed magnetic fields of up to 60 T, applied parallel to the tube axis. The accuracy of the alignment was $\pm$5° (see supplementary material for further experimental details).9

Figure 1(a) shows the magnetoconductance $G(B_0)$ of a small-band-gap CNT device located near the CNP (diameter $d \sim 1.5$ nm). At 82 K, the conductance $G$ of the tube initially increases to reach a maximum at $B_{||} = 5.9$ T, then it exponentially drops to zero at higher fields due to the Aharonov-Bohm (AB) effect.5,10 Interestingly, when the device was

![Graph showing magnetoconductance](image)

FIG. 1. (Color online) (a) MC of a small-band-gap CNT device near the CNP measured at 82 and 4.2 K. The inset shows the MC in a semilog scale. The observed double peak in $G(B_0)$ defines the characteristic fields $B_{11}^*$, $B_{11}$, and $B_2$. (b) One of the Dirac cones near the K points, intersected by lines of allowed $k_z$ values for a small-band-gap CNT with SOI. Spin-up and spin-down bands (marked by arrows) display a curvature-induced band gap $E_{\text{curv}}$ and are separated by $\Delta_{SO}$ due to the SOI. With increasing $B_{||}$, spin-split subbands shift due to the AB effect and cross the $K(K')$ point, successively closing the energy gap at $B_1$ and $B_2$. For simplicity, the Zeeman term and $\epsilon_{SO}$, an additional Zeeman-type term induced by the SOI, are neglected. However, $B_1$ and $B_2$ are not affected by those terms (see supplementary material) (Ref. 9).
cooled down to 4.2 K, the conductance maximum $G_{\text{max}}$ at $B_0$ was split into two distinct peaks at magnetic fields $B_1 = 3.1$ T and $B_2 = 11.1$ T. We note that these peaks are symmetric with respect to the conductance dip at $B_0^0 \approx 7$ T, and $G(B_0^0)$ is similar in magnitude to $G(B_0=0)$. The key to the explanation of the data lies in the magnetic field dependence of the one-dimensional band structure.

A specific CNT is uniquely labeled by the chiral indices $(n,m)$, which define the chiral angle $\theta$ and the quantized values of the transversal wave vector $k_0$. The values of $k_0$, combined with the graphene dispersion cones, determine the quasi-one-dimensional band structure of the CNTs. A given CNT is metallic if the lines of allowed $k_0$ cross the Dirac points $K$ and $K'$; otherwise it is semiconducting. For nominally metallic CNTs $(n−m=3l$, with $l$ an integer), the dispersion relation $E(k_0)$ near the Dirac points reads,

$$E(k_0) = \pm \hbar v_F\sqrt{k_0^2 + k_{\perp}^2} + \frac{g}{2} \mu_B B_1 + \tau \delta_{SO},$$

$$k_\perp = k_{AB} + k_{k_0} + k_{SO},$$

where $k_0$ is the wave vector parallel to the tube axis, $v_F$ the Fermi velocity, $\frac{g}{2} \mu_B B_1$ the Zeeman term with $\tau = \pm 1$ for spin parallel/antiparallel to the tube axis, and $\tau = \pm 1$ for the $K$ and $K'$ Dirac points. The transversal wave vector $k_{\perp}$ contains three distinct contributions, which are discussed below.

The Aharonov-Bohm flux $\psi_{AB} = B_1 \pi d^2/4$ results in a shift $k_{AB} = (2/d)(\psi_{AB}/\phi_0)$ of $k_0$, where $\phi_0 = h/e$ is the flux quantum. Therefore, one can convert a metallic CNT into a semi-one-dimensional band structure of the CNTs. A given band of the one-dimensional band structure.

For a conservative confidence interval of $\pm 0.5$ nm for $d$ determined with an atomic force microscope, one obtains $0.76 < \psi_{AB}/\phi_0 < 3$ compatible with previous studies. Equations (1)–(3) result in the energy splitting $\Delta_{SO}$ at $B_1=0$ (assuming $k_0=0$),

$$\Delta_{SO} = \frac{4\hbar v_F \phi_{SO}}{d \phi_0} = 2.5 \pm 0.8 \text{ meV}.$$

This value corresponds to $\sim 30$ K and explains the disappearance of the double-peak structure and the single conductance maximum at $B_1=0$ for the 82 K trace of Fig. 1. Because $\Delta_{SO}$ is inversely proportional to the diameter, it becomes large for small-diameter tubes.

With further increase in $\psi_{AB}$, the energy gap $E_g$ linearly opens again as both orbital subbands gradually move away from the conductance point of the Dirac cone. The exponential decrease in $G$ at high fields [the inset of Fig. (a)] is thus explained by charge carriers thermally activated over the magnetic-field-induced band gap, as described by previous authors. Since the inset in Fig. (a) suggests that the conductance depends exponentially on the band gaps $E_g$ and $E_{\text{curv}}$, they dominate the conductance at $B_1=0$ and $B_1=B_0'$. Hence, the approximate equality $G(0) \approx G(B_0')$ inferred from Fig. (a) suggests the following relation between the two energy scales $E_{\text{curv}}$ and $\Delta_{SO}$:

$$E_g^0 = E_{\text{curv}} - \Delta_{SO}.$$
FIG. 2. (Color online) (a) Calculated density of states in a parallel magnetic field for the (12,9) CNT. (b) Zoom into the area bounded by the gray box clearly shows that the band gap is closed at $B_1$ and $B_2$ in good agreement with the peak positions observed in Fig. 1(a). White arrows indicate the spin polarization of the bands near the crossing points $B_1$ and $B_2$. (c) DOS calculated for the (17,2) CNT. Due to the larger curvature-induced band gap of the (17,2) tube with $\theta$ close to 0$^\circ$, the Zeeman-energy splitting at $B_0/(g\mu_B B_0)=3.7$ meV is larger than the spin-orbit energy splitting ($\Delta_{SO}$=2.33 meV). Hence, the SOI-induced peak splitting is pronounced for the CNTs with chiral angles close to 30$^\circ$. Orbital ($K$ and $K'$) and spin states (white arrows) are indicated.

We now turn to the discussion of the effect of tube chirality. The strong dependence of $B_0$ and $B_0'$ on the chirality can be used to identify the chiral indices of small-band-gap CNTs. Out of 53 small-band-gap CNTs with $d=1.5 \pm 0.5$ nm, only five tubes [(12,9), (13,10), (16,10), (18,9), and (19,10)] display values of $B_0=5$–8 T compatible with our data while $B_0$ can take much larger values for other CNTs, e.g., the (12,3) and (17,2) tubes.

Table I lists values of $\phi_{SO}$ and $\Delta_{SO}$ for these chiralities, calculated from Eqs. (3) and (4) and the observed $\Delta B=8$ T. The $\phi_{SO}$ of the (12,9) tube is closest to $\phi_{SO}=10^{-3}\phi_0$, predicted in Ref. 12 and measured in Ref. 4. When we further take into account the condition $E_{curv}=2\Delta_{SO}$ for the CNT measured [Eq. (5)], we realize that the (12,9) and (18,9) tubes satisfy this constraint best.

Taking the (12,9) tube with the chiral angle $\theta=25.3^\circ$ (close to the armchair configuration) as the most probable candidate, we calculated the density of states (DOS) in a parallel magnetic field. We used the periodic boundary conditions, which are suitable for very long nanotubes. In shorter CNTs the open boundary condition in the axial direction gives rise additionally to edge effects, which are, however, beyond the scope of this work. For comparison, we show the DOS of a (17,2) tube, which has almost the same diameter but a very different chiral angle $\theta=5.5^\circ$ close to the zigzag configuration.

From Fig. 2, it becomes apparent that in an applied magnetic field the band edges change with four distinct slopes away from the two Kramers doublets both in the electron and hole bands, reflecting the orbital and Zeeman splitting. The DOS calculated for the (12,9) tube explains the evolution of the magnetoconductance very well. The band gap is closed at $B_1$ by the spin down and subsequently at $B_2$ by the spin-up subband, in very good agreement with the observed double peaks at the CNP. The calculated energy gaps at zero field and at $B_0'$ agree with Eqs. (4) and (5). On the other hand, the DOS calculated for the (17,2) CNT predicts a significantly reduced intermediate gap region in Fig. 2(c), in spite of almost the same $d$ and $\Delta_{SO}$, when compared with the (12,9) tube. The (17,2) tube has a much larger curvature-induced gap $E_{curv}=18.5$ meV, resulting in a much higher $B_0$.

FIG. 3. (Color online) (a) $G(B_0)$ traces at 4.2 K for the hole side of the CNP. As the band gap grows with $B_0$ at high fields, the gate characteristic $G(V_g)$ exhibits the behavior of a $p$-type CNT field-effect transistor with on-off conductance ratio of several orders of magnitude. The inset shows $G(V_g)$ at $B_0=0$. The dots correspond to the traces of $G(B_0)$ in main figure. The black solid line in the inset is a fit to experimental points (see error bar) given as a guideline to the eyes. (b) $G(B_0)$ curves for the electron side of the CNP. The double-peak structure is observed only when the Fermi energy is tuned close to the CNP at $V_g=+6$ V.
≈ 31.6 T. Because the spin-orbit gap competes with the Zeeman splitting, the peak splitting in $G(B_\parallel)$ is most pronounced for near armchair tubes with chiral angles close to 30°.

So far, all our discussion focused on the vicinity of the charge-neutrality point. As a crucial test of our analysis, we traced the evolution of the $G(B_\parallel)$ curves for various values of gate voltage. In Fig. 3(a), magnetoconductance traces at 4.2 K are displayed for the hole side of the CNP. Deeply inside the hole band, the conductance exceeds $3e^2/h$, close to the theoretical limit of $4e^2/h$. This shows that our device is in the ballistic regime, where the conductance is determined by the number of available subbands with an average transmission probability of $\sim 0.8$. At $B_\parallel = 0$, the hole conductance is around $3e^2/h$ and diminishes down to $\sim 0.5e^2/h$ as $E_F$ is tuned toward the CNP ($V_g \approx +6$ V). While the magnetoconductance is initially positive at low fields, it becomes negative at high fields ($B_\parallel \gg B_0$) for all gate voltages, indicating the growth of $E_F$ due to the AB effect. At $B_\parallel > 30$ T, the gate characteristic $\delta G(V_g)$ exhibits the behavior of a p-type CNT field-effect transistor with an on-off conductance ratio $\sim 10^3$.

The double-peak structure is pronounced only in the vicinity of the Fermi energy. In Fig. 3, for near armchair tubes with chiral angles close to 30°, the growth of the number of available subbands with an average transmission probability of $\sim 0.8$. At $B_\parallel = 0$, the hole conductance is around $3e^2/h$ and diminishes down to $\sim 0.5e^2/h$ as $E_F$ is tuned toward the CNP ($V_g \approx +6$ V). While the magnetoconductance is initially positive at low fields, it becomes negative at high fields ($B_\parallel \gg B_0$) for all gate voltages, indicating the growth of $E_F$ due to the AB effect. At $B_\parallel > 30$ T, the gate characteristic $\delta G(V_g)$ exhibits the behavior of a p-type CNT field-effect transistor with an on-off conductance ratio $\sim 10^3$.

The double-peak structure is pronounced only in the vicinity of the CNP ($+5.6 \leq V_g \leq +6.4$ V). Two additional $G(B_\parallel)$ curves, presented in Fig. 3(b), show that the two peaks merge again into one as $E_F$ is shifted to the electron side across the CNP.

Approximating the backgate coupling to the Fermi-energy shift as $\Delta E_F = 0.7 \times 10^{-3}\Delta V_g$ the DOS calculation matches the gate voltages in Fig. 3. For instance, the conductance kinks observed at 8 and 24 T for the $G(B_\parallel)$ curve at $V_g = -5.3$ V in Fig. 3(a), may be explained by the subsequent loss of $K'_\parallel$ subbands at $B = 8$ T and $K'_\parallel$, $K'_\parallel$ at $\approx 24$ T in the DOS. However, as the calculation neglects quantum interference effects in the Fabry-Perot regime, such as the AB beating effect, we cannot expect to explain all features of the measured magnetoconductance within our simple model.

In conclusion, we have investigated single-walled carbon nanotubes up to very high magnetic fields. The magnetoconductance of a quasimetallic tube shows a peculiar double peak, which can be explained in terms of spin-split conduction bands, separated by a strong spin-orbit interaction, which exceeds the Zeeman splitting. Our finding may open the path toward the application of CNTs as highly efficient ballistic spin filters.

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23 Therefore, $\Delta_{00}$ is larger for our nanotube, compared to the value observed for the tube ($d \approx 5$ nm) in Ref. 4.
