Magnetoresistance devices based on single-walled carbon nanotubes

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We demonstrate the physical principles for the construction of a nanometer-sized magnetoresistance device based on the Aharonov-Bohm effect [Phys. Rev. **115**, 485 (1959)]. The proposed device is made of a short single-walled carbon nanotube (SWCNT) placed on a substrate and coupled to a tip/contacts. We consider conductance due to the motion of electrons along the circumference of the tube (as opposed to the motion parallel to its axis). We find that the circumference conductance is sensitive to magnetic fields threading the SWCNT due to the Aharonov-Bohm effect, and show that by retracting the tip/contacts, so that the coupling to the SWCNT is reduced, very high sensitivity to the threading magnetic field develops. This is due to the formation of a narrow resonance through which the tunneling current flows. Using a bias potential the resonance can be shifted to low magnetic fields, allowing the control of conductance with magnetic fields of the order of 1 T.
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Understanding nanoscale electronic devices is intertwined with the ability to control their properties. One of the most scientifically intriguing and potentially useful property is the control of the electrical conductance in such devices.[1,2] A convenient way of affecting the conductance is by applying magnetic fields. In mesoscopic systems, for example, the conductance is sensitive to the Aharonov-Bohm (AB) effect.[3] The study of the interplay between bias and gate voltages, and magnetic fields in these systems has lead to the development of micronic AB interferometers.[4–6] At the nanoscale, however, it is widely accepted that AB interferometers do not exist.[7] This is because unrealistic huge magnetic fields are required to affect the conductance through a loop encircling very small areas (for a loop of area A, the magnetic field B needed to complete a full AB period can be obtained from the relation $AB=\phi_0$, where $\phi_0=h/e$ is the flux quantum, and h and e are Planck's constant and electron charge, respectively). Thus, at the nanoscale, devices that exhibit large magnetoresistance have been demonstrated based on the Zeeman spin splitting of individual molecular states,[8] or based on the Kondo effect.[9]

Therefore, an open question is whether one can devise a nanometric system that will exhibit large magnetoresistance at low magnetic fields utilizing the AB effect. Recently, the AB effect has been measured for single-walled and multi-walled carbon nanotubes (SWCNT and MWCNT, respectively).[10–12] The MWCNT with a relatively large diameter (15 nm) exhibits h/e-period magnetic-flux dependence with $B=5.8$ T for a full AB period. This result is important, showing that transport is coherent through the tube, in agreement with previous observations.[13] Furthermore, the measurements for the smaller diameter SWCNT indicate that the band structure of the tube depends on the magnetic flux threading it.[12] But, a full AB period and, thus, switching capability, would require magnetic fields of the order of 1000 T for a 1-nm-diameter SWCNT, much higher than those used in the experiment ($B_{\max}=45$ T).

In this Letter, we lay out the simple physical principles required to answer this question. Utilizing the AB effect, we suggest a way to switch the conductance through the nanometric cross section of a SWCNT by the application of low (≈ 1 T) magnetic fields parallel to the axis of the tube. Our scheme also provides a framework to study and control coherent transport in SWCNTs.

The main idea is that when a magnetic field is applied perpendicular to the cross section of the tube (along its main axis), electron pathways transversing the circular circumference in a clockwise and a counterclockwise manner gain different magnetic phases, and thus AB interference occurs. As the coupling between the CNT and the conducting leads is decreased, a resonant tunneling junction forms. This results in an increase of the electron's lifetime on the CNT and thus in a narrowing of the energy-level width. Using a bias/gate potential it is possible to tune the resonance such that the transmittance is high at zero magnetic field. The application of low magnetic fields shifts the narrow energy level out of resonance. Thus, switching accrues at fields much smaller than those required to achieve a full AB cycle.[7]

Two different experimental configurations are considered for this purpose. The first consists of a SWCNT placed on an insulating substrate between two thin conducting contacts [see Fig. 1(a)] and a bias potential is applied between the contacts. Similar setups have been recently demonstrated experimentally.[14–17] In the second configuration a SWCNT is placed on a conducting substrate coupled to a scanning tun-

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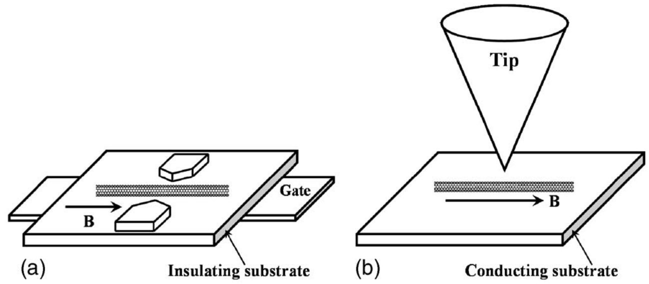

FIG. 1. An illustration of the expesrimental configurations suggested for measuring the cross-sectional magnetoresistance of a CNT. (a) The SWCNT is placed on an insulating surface between two narrow metallic contacts. (b) The SWCNT is placed on a conducting substrate and approached from above by a STM tip.

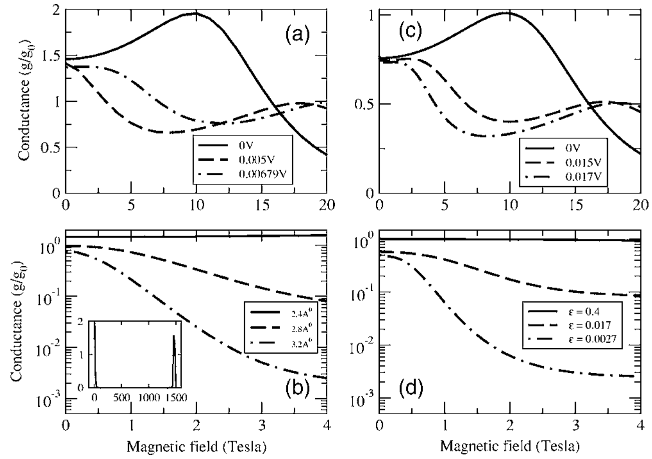

FIG. 2. Conductance vs the magnetic field for a (24,0) SWCNT computed for configuration (a). Panel a: MEHT results for the effect of a bias potential on the position of the conductance peaks at a constant tube-contact separation of 2.4 Å. Panel b: MEHT results for the effect of an increase in the tube-contact separation at a constant bias potential of 0.00679 V. Panel c: Continuum model results for the effect of a bias potential on the position of the conductance peaks for $\epsilon = 0.035$. Panel d: Continuum model results for the effect of a decrease in the junction transmittance amplitude ϵ at a constant bias potential of 0.0195 V. Inset of panel b: the full AB period for a (24,0) SWCNT at zero bias potential and tube-contact separation of 2.4 Å.

neling microscope (STM) tip from above, as described schematically in Fig. 1(b). The bias potential is applied between the STM tip and the underlying surface. For both configurations we calculate the resulting conductance between the leads, showing that high sensitivity on the magnetic field can be achieved.

To calculate the conductance of these systems in the presence of a uniform magnetic field, we have developed a simple approach based on the magnetic extended Hückel theory (MEHT).[7] Within this approach, we add the proper magnetic terms to the extended Hückel (EH) (tight binding) Hamiltonian, $\hat{H}_{\mathrm{EH}}$ (from now on we use a.u., unless otherwise noted):

$$\hat{H} = \hat{H}_{\mathrm{EH}} - \mu_B \hat{\mathbf{L}} \cdot \mathbf{B} + \frac{B^2}{8} R_{\perp}^2 . \tag{1}$$

Here $\mu_B = \frac{1}{2}$ is the Bohr magneton in a.u., $\hat{\mathbf{L}}$ is the angular-momentum operator, $\mathbf{B}$ is the magnetic-field vector, and $\mathbf{R}_{\perp}$ the projection of $\mathbf{R}$ onto the plane perpendicular to $\mathbf{B}$. A gauge invariant Slater-type orbitals (GISTO) basis set is used to evaluate the MEHT Hamiltonian matrix:

$$|\mathrm{GISTO}\rangle_{\alpha} = |\mathrm{STO}\rangle_{\alpha} e^{-(ie/\hbar)\mathbf{A}_{\alpha}\cdot \mathbf{r}}, \tag{2}$$

where $|\mathrm{STO}\rangle_{\alpha}$ is a Slater-type orbital centered on atom α, and $\mathbf{A}_{\alpha}$ is the vector potential evaluated at the nuclear position $\mathbf{R}_{\alpha}$, $\mathbf{A}_{\alpha} = -\frac{1}{2}(\mathbf{R}_{\alpha} \times \mathbf{B}_{\alpha})$. For the results reported below, all carbon atoms of the tube were treated explicitly. In the MEHT, each carbon atom contributes two s electrons and two p electrons. The valence s and p atomic orbitals are explicitly considered in the Hamiltonian. For configuration (a) [Fig. 1(a)] both leads are modeled by atomic conducting wires, while for configuration (b) [Fig. 1(b)] the STM tip is modeled by a semi-infinite, one-dimensional, atomic-conducting gold wire and the substrate is modeled by a semi-infinite slab of gold crystal. The calculations were conducted for a tube four unit cells in length,[18] using minimum image periodic boundary conditions for the passivation of the edge atoms. Tests on longer tubes reveal the same qualitative picture described below. We assume a homogeneous magnetic field parallel to the tube axis and calculate the Hamiltonian matrix elements analytically[19] within the Pople approximation.[20]

The conductance is calculated using the Landauer formalism[21] which relates it to the scattering transmittance probability through the system. The transmittance is given by $T(E) = 4tr[\hat{G}^{\dagger}(E)\Gamma_1(E)\hat{G}(E)\Gamma_2(E)]$. Here, $\hat{G}(E) = [E - \hat{H} + i(\Gamma_1 + \Gamma_2)]^{-1}$ is the retarded Green function and $\Gamma_{1/2}$ are the imaginary parts of the self-energy (Σ) of the left/right contacts or STM tip/substrate for the two measuring configurations, respectively. For the results represented below we use both imaginary absorbing potentials[22] and an iterative semi-infinite bulk Green's-function calculation scheme[23–25] to calculate the self-energies of the leads.

In Fig. 2, the conductance through the cross section of a (24,0) SWCNT, calculated for configuration (a), is plotted against the external axial magnetic field applied. In panel (a) we plot the conductance as a function of the axial magnetic field at low values of the field, and for several values of the bias potential. The conductance at zero bias first increases as we switch on the magnetic field (negative magnetoresistance), peaks near $B = 10$ T, and subsequently decreases as the field grows, vanishing at fields above 30 T. The maximum conductance observed, $g/g_0 = 2$, is limited by the number of open channels in the vicinity of the Fermi energy of the SWCNT. In order to achieve switching capability at magnetic fields smaller than 1 T, it is necessary to move the conductance peak to zero magnetic fields and at the same time reduce its width.

When a small bias is applied to the sample the conductance peak splits into a doublet. The position of the corresponding peaks depends on the value of the bias and the maximum conductance is reduced by 25%–50%. As can be seen in the figure, by adjusting the bias potential it is possible to shift one of the conductance peaks toward low values of the magnetic field, such that the conductance is maximal at $B = 0$ T and positive magnetoresistance is achieved. The

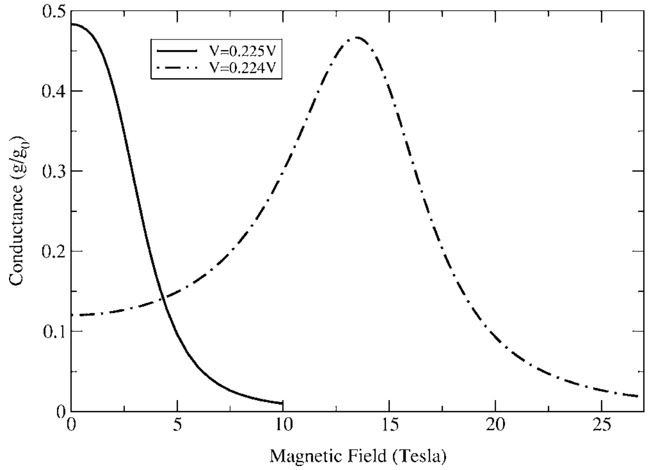

FIG. 3. Conductance as a function of the magnetic field through a (6,0) CNT as calculated for configuration (b).

shift in the conductance peak can be attributed to the change in the energy level through which conductance occurs when a small bias is applied. As a result of this change, the electron momentum changes and this leads to a shift seen in the conductance peak.

In Fig. 2(b), the effect of changing the tube-contact separation at constant bias potential is studied. As one increases the separation between the tube and the contacts, their coupling decreases, resulting in a reduction of the width of the energy resonances of the SWCNT. Thus, the conductance becomes very sensitive to an applied magnetic field and small variations in the field shift the relevant energy level out of resonance. In the magnetoresistance spectrum, this is translated to a narrowing of the transmittance peaks. For the smallest separation considered (2.4 Å), the conductance seems to be constant, on the logarithmic scale, at the magnetic-field range shown in the figure, while at the highest separation studied (3.2 Å), the width of the conductance peak is comparable to 1 T. At higher magnetic fields (not shown) the conductance of the 2.4-Å case reduces as well.

Considering the combined effect of the bias potential and the tube-contact separation, it is possible to shift the position of the conductance peak to small magnetic fields while at the same time reduce its width. This is achieved by carefully selecting the values of the bias potential and tube-contact separation. Under proper conditions, we obtain positive magnetoresistance with a sharp response occurring at magnetic fields comparable to 1 T. This result is significant since it implies that despite the fact that the tube radius is small ($\sim$1 nm) and the corresponding full AB period requires unrealistic large magnetic fields of the order of 1500 T [as shown in the inset of Fig. 2(b)], it is possible to achieve magnetic switching at relatively small magnetic fields.

A similar picture arises when considering configuration (b). In Fig. 3 we plot the conductance as calculated for a (6,0) SWCNT placed between a sharp STM tip and a conducting surface for two bias voltages. We use a smaller diameter CNT in these calculations in order to be able to properly describe the bulky nature of the conducting substrate with respect to the dimension of the CNT. The separation between the CNT and the conducting leads used in this calculation is taken to be 4.1 Å.

As can be seen, when a bias voltage of $\sim$0.224 V is applied, the conductance peaks at a magnetic field of $\sim$14 T. By changing the bias potential to $\sim$0.225 V the conductance peak shifts toward zero magnetic field. Under these conditions switching occurs at a magnetic field of $\sim$10 T while the full AB period for this system is of the order of 2×10^4 T. The CNT-lead separation required to achieve high magnetoresistance sensitivity in this configuration is larger than the one needed for configuration (a). This is due to the difference in the CNT diameters and the different lead geometries. As the diameter of the tube becomes smaller, the magnetic field needed to gain a similar AB phase shift grows larger. Thus, the conductance peaks become wider and larger CNT-lead separations are needed in order to narrow their width. Furthermore, as the lead becomes more bulky its coupling to the CNT needs to be decreased in order to achieve the same magnetoresistance sensitivity.

As discussed in our previous work,[7] the results described above can be reproduced by a simple one-dimensional (1D) continuum model. The model consists of a continuum loop coupled to two continuum wires and placed in a perpendicular magnetic field. The electron is considered to ballistically transverse the wires and the ring while elastic scattering occurs at the junctions. The transmittance probability for an electron originating at one wire to emerge at the other wire can be calculated exactly as a function of the magnetic field.[26,27] Two independent parameters control the shape of the magnetotransmittance diagram: the wave number, k, of the conducting electron and the probability amplitude, ϵ, of an electron approaching the junction from the leads to be transmitted into the ring. In panels c and d of Fig. 2 we present the results of the continuum model for a ring of radius $R=9.5255$ Å and electron wave number approximately equal to that of a Fermi electron in a graphene sheet ($k=2\pi/3.52$ Å^{-1}). As can be seen in panel c, changing the bias potential results in a shift in the position of the transmission peaks similar to the effect seen in the MEHT atomistic calculations (panel a). Furthermore, in panel d we present the effect of reducing the in-scattering probability at the junction which results in a narrowing of the conductance peaks. This corresponds to reducing the coupling (increasing the separation) between the leads and the ring in the MEHT atomistic calculations (panel b). Although the 1D model does not poses the full three-dimensional (3D) characteristics of the CNT we find that it captures all the essential physics to reproduce the results of the conductance through such a complex system. The only fitting parameter is the ring-leads transmittance amplitude.

The above calculations for the (24,0) CNT assume a low temperature of 1 K. However, the effects we report will hold even at higher temperatures. The temperature T must be low enough to resolve the magnetic-field splitting of circumference energy levels, and thus satisfy[7] $k_B T < [\hbar^2 k_f / m^* D] \times [\phi/\phi_0]$. Here D is the diameter of the tube, k_f is the Fermi wave number, and m^* is the electron's effective mass. For a ratio of $[\phi/\phi_0]=1/1500$ (namely, switching capability at 1

T) the upper limit for the temperature is ~20 K. Due to the small diameter of the (6,0) CNT the temperature used for the calculations of configuration (b) was 0.1 K. However, for a larger diameter CNT, such as the (24,0) CNT used in the calculations of configuration (a), similar results are expected at higher temperatures.

In summary, we have demonstrated that SWCNTs can be used as magnetoresistance switching devices based on the AB effect. The essential procedure is to weakly couple the SWCNT to the conducting leads in order to narrow the conducting resonances, while at the same time to control the position of the resonances by the application of a bias potential. The control over the coupling between the SWCNT and the conducting leads in configuration (a) of Fig. 1 can be achieved via a fabrication of a set of leads with proper gaps. In configuration (b) of the same figure one needs to control the distance between the STM tip and the CNT and between the substrate and the CNT. The former can be achieved by piezoelectric control and the latter can be controlled by covering the surface with monolayer/s of an insulating material. The fact that the diameter of the tube is small becomes beneficial, since the separation between the circumferential energy levels on the tube is large. Therefore, conductance can be achieved through a single, well-defined state and is thus less sensitive to temperature effects. The advantage of using a magnetic field in nanometer scale AB interferometers was recently demonstrated for multichannel devices where the polarity of the magnetic field can selectively control the outgoing channel.[28] This is due to the symmetry-breaking nature of the magnetic field.

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