Carbon nanotube: A low-loss spin-current waveguide

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(Received 24 March 2010; published 19 April 2010)

We demonstrate with a quantum-mechanical approach that carbon nanotubes are excellent spin-current waveguides and are able to carry information stored in a precessing magnetic moment for long distances with very little dispersion and with tunable degrees of attenuation. Pulsed magnetic excitations are predicted to travel with the nanotube Fermi velocity and are able to induce similar excitations in remote locations. Such an efficient way of transporting magnetic information suggests that nanotubes are promising candidates for memory devices with fast magnetization switchings.

DOI: 10.1103/PhysRevB.81.153408 PACS number(s): 73.63.Fg, 72.25.Ba, 75.30.Hx, 75.75.−c

The issue of magnetization dynamics in low-dimensional systems is currently one of the most studied in spintronics.[1] In particular, controlling how quickly the energy of a precessing magnetic moment propagates through wires is motivated by the possibility of building miniaturized memory devices with fast magnetization switchings. This requires structures functioning as efficient spin-current waveguides, i.e., conduits capable of transporting spin information with little attenuation. Renowned for their high thermal and electronic conductivities, for their long aspect ratios and coherence lengths, carbon nanotubes (NT) possess the ideal characteristics for acting as waveguides. NT have indeed been shown to function as conduits for electrons[2,3] and for phonons.[4] A natural question to ask, raised in this Brief Report, is whether these materials are also efficient spin-current waveguides.

Tserkovnyak[5,6] proposed a mechanism for pumping spin current into a nonmagnetic metal caused by the precession of an adjacent magnetization. In this case, angular momentum from the moving magnetization is transferred to the conduction electrons, creating a spin disturbance that propagates throughout the metallic conduit. This spin flow is produced without an applied voltage, involves no net electrical current, and may be used to excite other magnetic units also in contact with the nonmagnetic metal. Our strategy is to test this mechanism with NT in contact to local magnetic moments.

Obstacles for identifying good spin waveguides lie in the difficulties of predicting the precise time evolution of the magnetization of a realistic system, taking into consideration the details of its electronic structure. This requires a full understanding of how a pulsed magnetic excitation evolves. Although previously treated semiclassically[5,6] and quantum mechanically,[7,8] a time-dependent quantum approach for this problem is still missing. In this Brief Report we bridge this gap and provide a quantum formalism that describes in time domain how a localized magnetic perturbation propagates throughout a nanoscale system, more precisely a metallic NT. In doing so, we are able to show that NT are excellent spin-current waveguides. We demonstrate that they transport spin current across long distances in a dispersionless fashion and with little attenuation. Moreover, we indicate that pulsed spin excitations propagate with a characteristic speed given by the electronic Fermi velocity and with a tunable degree of attenuation that depends on the excitation frequency.

We consider a metallic NT doped with a single substitutional magnetic impurity,[9,10] as depicted in the inset of Fig. 1. Assuming the existence of a localized magnetic moment pointing along the $\hat{z}$ direction, we consider a perturbing time-dependent transverse magnetic field $\vec{h}_{\perp}(t)$ which sets the impurity magnetic moment into precession. Our treatment applies to magnetic moments at temperatures above their Kondo temperatures which are nevertheless expected to be quite low in NT. We assume the Fermi-liquid representation and do not include any Luttinger-liquid effects.[11] To determine whether a NT is a good conduit for spin currents, we must assess how such a localized magnetic excitation propagates across the structure. In other words, we must investigate how this excitation disturbs the spin balance of the system not only where the impurity is located but also, and more importantly, how the local spin dynamics is affected away from the impurity. This is naturally manifested by the spin susceptibility χ, which reflects how the spin degrees of freedom of a system responds to a magnetic excitation.

To calculate the spin susceptibility one needs the Hamiltonian describing the electronic structure of the unperturbed system, which we assume is given by $\hat{H}=\Sigma_{\langle i,j\rangle,\sigma}\gamma_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}+\Sigma_{\sigma}(\epsilon_0\hat{n}_{0,\sigma}+\frac{U}{2}\hat{n}_{0\sigma}\hat{n}_{0\bar{\sigma}})+\hat{H}_Z$. Here, γ_{ij} represents the electron hopping between nearest neighbor sites i and j, $\hat{c}^{\dagger}_{i\sigma}$ creates an electron with spin σ in site i, ϵ_0 is the atomic energy level of the magnetic impurity occupying the site $i=0$, $\hat{n}_{0\sigma}=\hat{c}^{\dagger}_{0\sigma}\hat{c}_{0\sigma}$ is the corresponding electronic occupation number operator, and U represents an effective on-site interaction between electrons in the magnetic site, which is neglected elsewhere. Finally, H_Z plays the role of a local Zeeman interaction that defines the $\hat{z}$ axis as the equilibrium direction of the magnetization. The Hamiltonian parameters can be obtained from density-functional-theory calculations so that the electronic structure of the doped system is well described.[12,13] Although we shall present results for a NT doped with Mn atoms, other substitutional magnetic impurities may be employed.[10] In our calculations we fix the Fermi energy $E_F=0$, and use $\gamma_{\mathrm{C,C}}=2.7$ eV, and $\gamma_{\mathrm{Mn,C}}=1.0$ eV. We take the number of d electrons in the Mn site $n_0=1$, $\epsilon_0=0$, $U=5$ eV, and assume a local Zeeman energy splitting $\delta_0=1$ meV. Spin-orbit coupling is neglected for being very small compared to the electronic bandwidth of NT.

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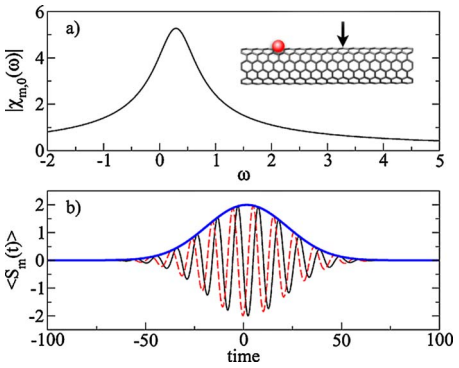

FIG. 1. (Color online) (a) Spin susceptibility $\chi_{m,0}$ (in units of $\hbar/\mathrm{eV}$) as a function of the excitation frequency ω (in terahertz) for a (4,4) NT. The distance between site m and the impurity is $x_m = 3a_0$. Inset shows NT with a single magnetic impurity. Arrow represents where the electrons spin is probed. (b) Solid and dashed lines represent the $\hat{x}$ and $\hat{y}$ components of the spin disturbance $S_m^+(t)$; the thick solid line depicts $|S_m^+(t)|$. Spins are in units of $\hbar g \mu_B h_0$, where g is the electron spin g factor, μ_B is the Bohr magneton, and h_0 is the amplitude of the applied time-dependent transverse field; time is given in picosecond. Results were generated with a Gaussian pulse centered at frequency $\omega = 0.6$ THz and with a standard deviation $\sigma = 20.7$ ps.

The time-dependent transverse spin susceptibility is defined as $\chi_{m,j}(t) = -\frac{i}{\hbar}\Theta(t)\langle[\hat{S}_m^+(t), \hat{S}_j^-(0)]\rangle$, where $\Theta(x)$ is the Heaviside step function, and $\hat{S}_m^+$ and $\hat{S}_m^-$ are the spin raising and lowering operators at site m, respectively. The indices j and m refer to the locations where the field is applied and where the response is measured, respectively. In our case, a precession of the magnetic moment is induced at site $j=0$, and we wish to observe the spin disturbance at an arbitrary site m. This response is fully described by $\chi_{m,0}(t)$. Within the random-phase approximation, this susceptibility may be calculated in frequency domain, and in matrix form it is given by $\chi(\omega) = [1 + \chi^0(\omega)U]^{-1}\chi^0(\omega)$, where χ^0 is the Hartree-Fock susceptibility, whose matrix elements are given by

$$\chi^0_{m,j}(\omega) = \frac{i\hbar}{2\pi}\int_{-\infty}^{+\infty} d\omega' f(\omega')\{[g^{\uparrow}_{j,m}(\omega') - g^{\uparrow *}_{m,j}(\omega')] \times g^{\downarrow}_{m,j}(\omega' + \omega) + [g^{\downarrow}_{m,j}(\omega') - g^{\downarrow *}_{j,m}(\omega')]g^{\uparrow *}_{m,j}(\omega' + \omega)\}. \quad (1)$$

Here, $g^{\sigma}_{m,j}(\omega)$ represents the time Fourier transforms of the retarded single-particle propagators for an electron with spin σ between sites m and j, and $f(\omega)$ is the Fermi function. For a pristine NT $g^{\sigma}_{mj}(\omega)$ may be analytically determined[14] and the integration in Eq. (1) performed with great numerical accuracy.

It is instructive to start by calculating $\chi_{m,0}(\omega)$ given by Eq. (1). A typical result is shown in Fig. 1(a) for a (4,4) armchair NT doped with a single Mn impurity. It depicts $|\chi_{m,0}(\omega)|$ which is proportional to the amplitude of the spin disturbance at site m due to a time-dependent transverse magnetic field applied at site 0. In Fig. 1(a) the site m is a distance $x_m = 3a_0$ from the impurity, where $a_0 \approx 2.46$ Å represents the graphene lattice parameter. A very distinctive peak is evident in the ω-dependent susceptibility, reflecting the existence of a resonance close to the Larmour frequency, as expected.

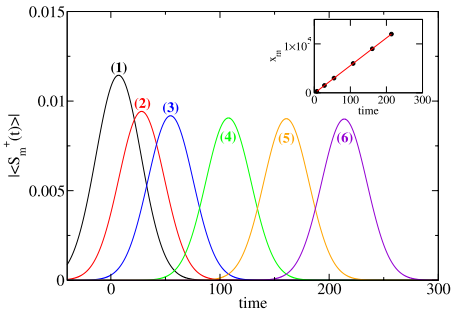

FIG. 2. (Color online) Amplitude of the transverse spin disturbance (in units of $\hbar g \mu_B h_0$) as a function of time (in picosecond) at different distances x_m from the magnetic impurity. The curves labeled from (1) to (6) represent signals probed at different values of $x_m = 0.3$, 1.5, 3, 6, 9, and $12 \times 10^4 a_0$, respectively. Inset plots how the corresponding probing positions x_m relate with the time τ taken to reach a maximum spin disturbance.

Since we are interested in studying the propagation of magnetic signals, it is illustrative to look at the susceptibility as a function of time rather than frequency. The Fourier transform of the curve depicted in Fig. 1(a) gives the spin disturbance response to an instantaneous δ-like pulse $\vec{h}_\perp(t)$ applied at site 0. However, for practical reasons, we consider the response to a Gaussian transverse magnetic field pulse given by $\vec{h}_\perp(t) = \vec{h}_0 \exp(-\frac{t^2}{2\sigma^2})$ applied along the $\hat{x}$ direction ($\vec{h}_0 = h_0\hat{x}$). Here h_0 represents the maximum field strength and σ its standard deviation. Figure 1(b) shows how such a magnetic pulse applied at the impurity location affects the spin balance of the NT at a nearby site ($x_m = 3a_0$). The thin solid and dashed lines represent the calculated spin components $\langle S_m^x(t)\rangle$ and $\langle S_m^y(t)\rangle$, respectively, and the modulating thick solid line is the magnitude of the transverse spin disturbance given by $|\langle S_m(t)\rangle| \equiv \sqrt{\langle S_m^x\rangle^2 + \langle S_m^y\rangle^2}$. To avoid congested figures the magnitude will be hereafter used to represent the spin dynamics on the NT.

The fact that the electron spin probed on the NT displays the precessional motion originated at the impurity is a clear indication of a flowing spin current emanating from the impurity into the NT. Earlier calculations have suggested that the existence of this current is sufficient to induce a dynamic magnetic coupling between dispersed impurities in NT, which is far more pronounced and long ranged than any other magnetic coupling of static nature.[7,8,14,15] To test how this precession propagates, in Fig. 2 we show $|\langle S_m(t)\rangle|$ probed at different locations on the NT. The six numbered lines correspond to spin disturbances probed at different sites along a line parallel to the NT axis containing the impurity site 0. The spin disturbance probed on other sites belonging to the same NT ring are virtually identical to the ones displayed in Fig. 2. Small deviations are noticeable when the ring is very close to the impurity but disappear after a short propagation distance. This indicates that the initial omnidirectional excitation produced by the applied perturbation

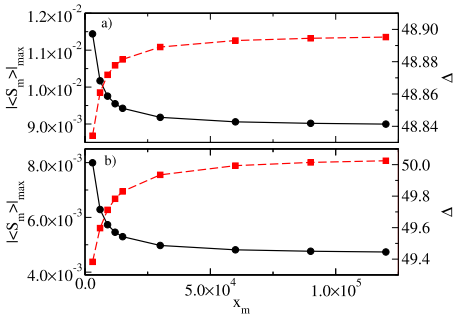

FIG. 3. (Color online) Left axis depicts maximum amplitude of the pulsed excitation $|\langle S_m\rangle|_{\max}$ (in units of $\hbar g\mu_B h_0$) probed at site m and is shown by the solid line with circular symbols. Right axis represents the width Δ (in picosecond) of the probed pulses shown by dashed lines with square symbols. Both quantities are plotted as a function of the separation x_m (in units of a_0) from the impurity location. Panels (a) and (b) are for pulses centered at resonance and off-resonance frequencies, respectively.

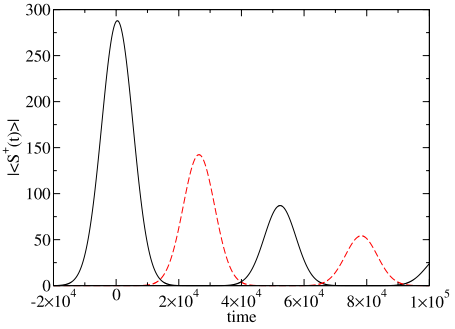

FIG. 4. (Color online) Amplitude of the pulsed excitation as a function of time (in picoseconds) for the case of two magnetic impurities a long distance apart ($x_m=6\times10^4a_0$). Solid line shows the spin disturbance evaluated at the impurity where the excitation is induced whereas the dashed line is evaluated at the other impurity location.

decays very fast into a cylindrical wave front that moves along the NT axial direction with a uniform speed. This propagation speed is found from the slope of the straight line in the inset of Fig. 2 showing the probing position x_m as a function of the time τ spent by the pulse maximum to reach x_m. We find the propagation velocity $v=1.4\times10^5$ m/s, which is precisely the NT Fermi velocity, indicating that the conduction electrons at E_F are the main carriers of the spin current.

Figure 2 shows that, as the pulse moves, it is initially deformed but it quickly reaches a form that remains unaltered for asymptotically long distances. This can be seen when we focus on two features of the pulsed signals, namely, their maximum amplitude $|\langle S_m\rangle|_{\max}$ and their corresponding width, here represented by the midheight separation Δ. Figure 3(a) plots $|\langle S_m\rangle|_{\max}$ and Δ as a function of the probing position x_m in the case of an excitation pulse whose frequency spectrum is centered at the same frequency as used for obtaining Fig. 1(b). Both quantities saturate after a short distance and are stationary for $x_m>10^4a_0$. This is a remarkable result showing that the information contained in the magnetic pulse can be transported across very long distances without distortion. Surely, the asymptotic value for $|\langle S_m\rangle|_{\max}$ is not the same as the one probed near the impurity but it still has a sizable magnitude indicating that a considerable fraction of the energy contained in the magnetization precession can be used elsewhere.

Furthermore, we can also control the fraction of the original pulse that reaches this asymptotic regime by selecting the central frequency in the excitation pulse. Figure 3(b) displays $|\langle S_m\rangle|_{\max}$ and Δ for the case of a pulse whose spectrum is centered at an off-resonance frequency $\omega=0.24$ THz. In this case the asymptotic value for $|\langle S_m\rangle|_{\max}$ is much reduced when compared with its counterpart in Fig. 3(a). The existence of this nondecaying asymptotic contribution to the spin current has been demonstrated recently for NT and atomic chains[7,8] but here we explicitly show that this can be actually controlled by an appropriate selection of excitation frequencies. All the features presented so far indicate that NT can carry spin-current information contained within pulsed excitations without dispersing their form. This can be explained by the peculiar electronic structure exhibited by NT, which is notoriously dispersionless at the Fermi level. In other words, extended states at the Fermi level have a linear dependence on the electronic wave vectors. In this case, group and phase velocities are interchangeable, meaning that every single frequency component comprising a pulse will travel with the same speed, thus preventing any distortion of the pulse shape. If NT are to be used as spin-current waveguides, these features must be tested in the presence of structural disorder. In fact, we have simulated the presence of isolated Boron substitutional impurities to explore their effect in the propagation of the spin disturbance pulse. We find that the pulse preserves its shape and amplitude, except very close to the B impurity, where it becomes slightly distorted. We notice that at larger distances, however, the pulse shape is restored as if no impurity is present. This suggests that the spin-current waveguide features reported so far are robust against the presence of nonmagnetic disorder in NT.

Finally, finding small values for the pulse amplitude at asymptotically large distances [see left axis of Figs. 3(a) and 3(b)] does not imply that the magnetic information is lost. To make this point more explicitly we add a second magnetic impurity a long distance from the original one ($x_m=6\times10^4a_0$) and see whether the excitation produced at the origin can be transported to the new location. Figure 4 shows the spin disturbance $|\langle S_m^+\rangle|$ probed on both impurities. The solid line shows the magnetization precession at the origin whereas the dashed line represents the spin disturbance as a function of time measured at the second impurity. Both lines have equally spaced peaks that are a time interval $\Delta t=2x_m/v$ apart but are shifted by half that amount. This is easily explained by the fact that precessing magnetic moments will always emit spin current to the surrounding conduction electrons which will induce further precessions when interacting with other magnetic moments. Therefore, the induced precession probed at the origin appears as the first peak in Fig. 4. The subsequent pulse is seen to occur after the spin current has traveled all the way to excite the second impurity at site m. Once excited, this impurity precesses also emitting spin current, which will again induce another pre-

cession at the origin. This process is repeated indefinitely each time with smaller amplitudes. The amplitude reduction is inevitable because half of the energy stored in the pulsed precession will travel away from the other impurity. But the fact that the pulse produced at the origin reappears a long distance apart means that the energy stored in the precession of magnetic moments can be noiselessly transported across the conduction electrons of NT, which confirms that these materials are ideal spin-current waveguides.

In summary, we have shown that metallic NT are excellent spin-current waveguides and are able to transport magnetic information across long distances with minimum dispersion and with very little loss. Spin disturbances induced by localized magnetic excitations are shown to propagate throughout the length of a metallic NT with speeds on the order of 10^5 m/s. Moreover, we show that the energy stored in a magnetic precession can be used elsewhere when the spin current traveling through NT interacts with other magnetic objects. These features turn NT into ideal components for fast-response memory devices. The experimental testing of our predictions requires the generation and detection of spin currents. One possibility is to excite a spin with a laser pulse and monitor a second spin located somewhere downstream with a scanning tunneling microscope (STM) tip. Since the STM current can be modulated by a coherent spin precession, one should be able to observe the second spin being excited by the spin current in the NT.

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