

Giant magneto-conductance in twisted carbon nanotubes

S. W. D. BAILEY¹, D. TOMÁNEK², Y.-K. KWON²(*) and C. J. LAMBERT¹

¹ *Department of Physics, Lancaster University - Lancaster, LA1 4YB, UK*

² *Department of Physics and Astronomy*

and Center for Fundamental Materials Research

Michigan State University - East Lansing, MI 48824-1116, USA

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Abstract. – Using the Landauer-Büttiker formalism, we calculate the effect of structural twist on electron transport in conducting carbon nanotubes. We demonstrate that even a localized region of twist scatters the propagating π electrons and induces the opening of a (pseudo-) gap near the Fermi level. The subsequent conductance reduction may be compensated by an applied axial magnetic field, leading to a twist-induced, giant positive magneto-conductance in clean armchair nanotubes.

Carbon nanotubes [1–3] exhibit a range of unusual electronic properties associated with the morphology of these quasi-1D structures. Early one-electron theories successfully associated metallic or semi-conducting behaviour with the chiral vector that characterizes a given nanotube [4–6]. Further studies addressed the effect of atomic-level impurities [7–10] and inter-tube interactions [11–14] on electrical conductance, or magneto-transport [7,15–19]. In parallel with the development of such one-electron theories, intensive studies of electron-electron correlations have been undertaken. Indeed, nonlinear current-voltage (I - V) characteristics have recently been observed [20], which are reminiscent of Luttinger liquid behaviour. An intriguing question remains however, namely whether other effects may augment or even dominate such nonlinearities in the transport properties of nanotubes.

In this letter we predict that scattering of electrons from twistons may give rise to strongly nonlinear I - V characteristics. Twistons [21–23], associated with regions of axial twist in otherwise perfect nanotubes, are intrinsic defects that are frozen into nanotube bundles during their synthesis and hence cannot be ignored when discussing electron transport. Unlike ideal straight and defect-free nanotubes, which have been shown to exhibit conventional magneto-resistive behaviour [24], we find that nanotubes containing twistons may behave in a very different way. In twisted tubes, we predict the occurrence of a giant positive magneto-conductance, an unexpected effect that by far exceeds the positive magneto-conductance associated with weak localisation in disordered tubes [25].

(*) Present address: Covalent Materials, Inc. - 1295A 67th Street, Emeryville, CA 94608, USA.

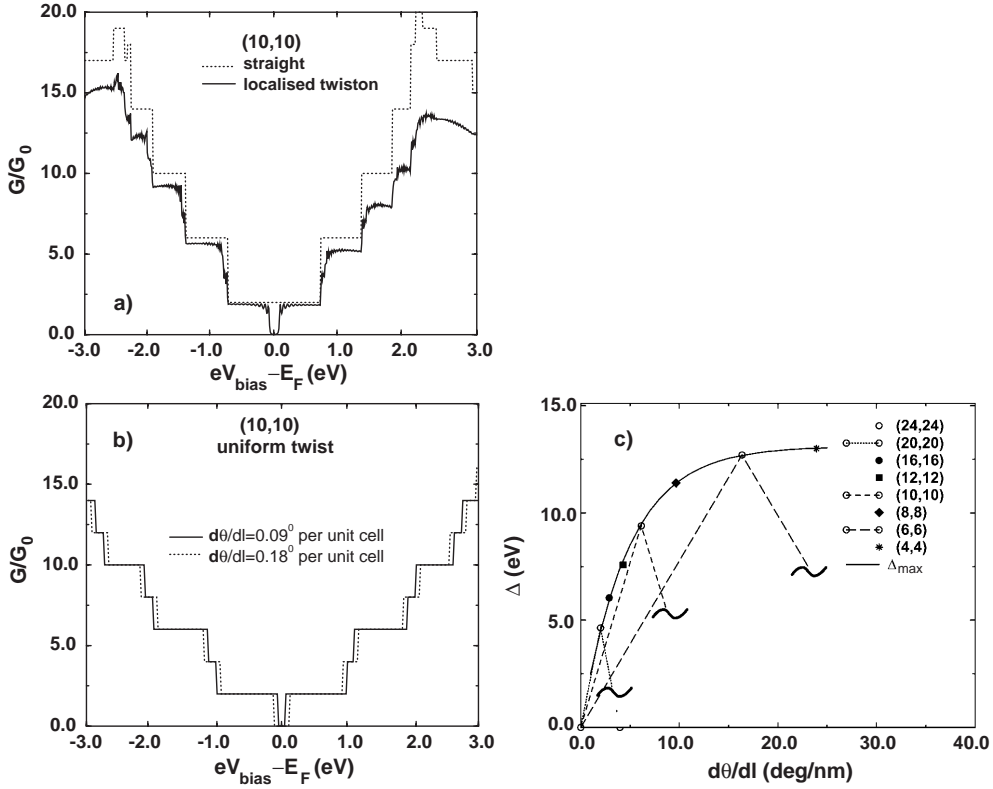


Fig. 1 – Differential conductance G of an infinite (10, 10) carbon nanotube as a function of the applied bias voltage V_{bias} . (a) Results for a perfectly straight tube (dotted line) are compared to those for a $\Delta\theta = 36^\circ$ finite twiston extending over 100 unit cells in the axial direction. For a tube with radius R , a portion of the unit cell of length L is shown in the inset. $G_0 = 2e^2/h$ is the conductance quantum. (b) Differential conductance of the (10, 10) nanotube subject to an infinitely long uniform twist, for different values of the twist per unit length $d\theta/dl$. (c) Dependence of the conductance gap Δ on the infinitely long twist $d\theta/dl$ for various (n, n) nanotubes.

To compute the effect of a finite scattering region on transport in an otherwise perfect (n, n) armchair nanotube, we use a parameterized four-state (s, p_x, p_y, p_z) Hamiltonian, based on a global fit to density functional results for graphite, diamond and C_2 as a function of the lattice parameter [26]. A finite twiston is treated as a scattering region connecting two semi-infinite (n, n) nanotubes. A recursive Green's function formalism is used to evaluate the transmission matrix \mathbf{t} , describing the scattering of electrons of energy E from one end of the semi-infinite nanotube to the other [27]. The differential electrical conductance at bias voltage V_{bias} is related to scattering properties at energy $E = E_F - eV_{\text{bias}}$ by the Landauer formula $G = G_0 \text{Tr} \{ \mathbf{t}^\dagger \mathbf{t} \}$, where $G_0 = 2e^2/h$ is the conductance quantum. A twiston is formed by introducing a small angular distortion between neighbouring axial slices within the scattering region. This is shown schematically in the inset of fig. 1(a), which displays the local shear distortion within the unit cell of length L , containing two axial slices. The perturbation to the Hamiltonian matrix enters through the scaling of the nearest-neighbour hopping integrals that follow the changes in C-C bonds \mathbf{r}_1 and \mathbf{r}_2 .

Figure 1 shows the differential conductance for a straight and twisted (10, 10) nanotube. In

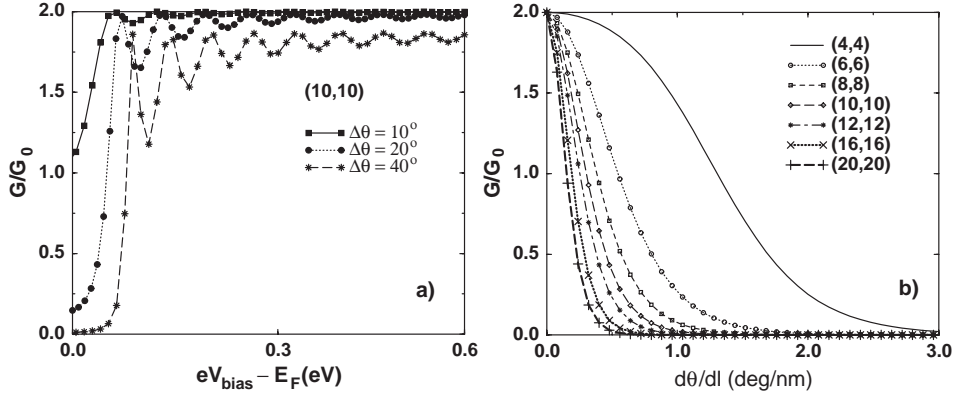


Fig. 2 – (a) Details of the differential conductance G of a (10,10) carbon nanotube subject to a finite twiston, as a function of the applied bias voltage V_{bias} . (b) Differential conductance of (n,n) nanotubes at zero bias as a function of the local twist in finite twistons. In both figures, the twistons $\Delta\theta$ extend only across a finite segment of 100 unit cells in the axial direction.

the straight nanotube of fig. 1(a), the nondegenerate bands, which cross near E_F , open up two conductance channels at this energy. Additional conduction channels follow as an increasing number of subbands appear near $E_F - eV_{\text{bias}}$ at higher bias voltages. In the presence of a localized twiston, the differential conductance is suppressed at all energies, in particular near the Fermi level. This is shown in fig. 1(a) for a finite-length twiston, with a total twist of 36° extending over 100 unit cells or ≈ 24.6 nm. The occurrence of a conductance gap near E_F suggests that electron scattering by a finite twiston can be viewed as a tunneling phenomenon.

For comparison with fig. 1(a), fig. 1(b) shows results for a nanotube subject to an infinitely long uniform twist $d\theta/dl$. This shows that that a localized or infinitely long twist opens up a conductance gap Δ near E_F . The predicted gap in the presence of infinitely long twists is shown in fig. 1(c) and agrees with results of refs. [21] and [22].

In the following, we discuss the dependence of the conductance gap on the twist distortion $d\theta/dl$, the spatial extent of the twiston, and an axially applied magnetic field. As shown in fig. 1(c), we find that for a range of (n,n) tubes subject to an infinitely long twist, the magnitude of the conductance gap Δ increases linearly with increasing twist distortion to its maximum value Δ_{max} , and decreases thereafter. For an (n,n) nanotube, we find the maximum value of the conductance gap Δ_{max} to be achieved at an “optimum tube twist” value $(d\theta/dl)_0 \approx An^{-2}$ (with $A = 620^\circ/\text{nm}$), which depends on the chiral index n . The dependence of Δ_{max} on the optimum tube twist $(d\theta/dl)_0$ corresponds to the envelope function in fig. 1(c), and is well approximated by $\Delta_{\text{max}} \approx \Delta(d\theta/dl)_0 \approx 1.30$ eV $(1 - e^{-0.21(d\theta/dl)_0})$, with $(d\theta/dl)_0$ in $^\circ/\text{nm}$ units.

Details of conductance changes due to localized twistons, such as those of fig. 1(a), are shown for small bias voltages in fig. 2(a). In the present case, we subjected a straight (10,10) nanotube to finite twists $\Delta\theta$ extending over 100 unit cells. We find that the conductance pseudo-gap associated with finite twistons is accompanied by conductance oscillations at small bias voltages. A tube subject to an infinitely long twist, on the other hand, possesses a real gap with no such oscillations. The zero-bias conductance as a function of the twist angle for finite twistons extending over 100 unit cells is presented in fig. 2(b) for a range of tube sizes. This type of conductance behaviour is reminiscent of that associated with tunneling through a potential barrier, where the twist-induced gap is analogous to the height of the barrier.

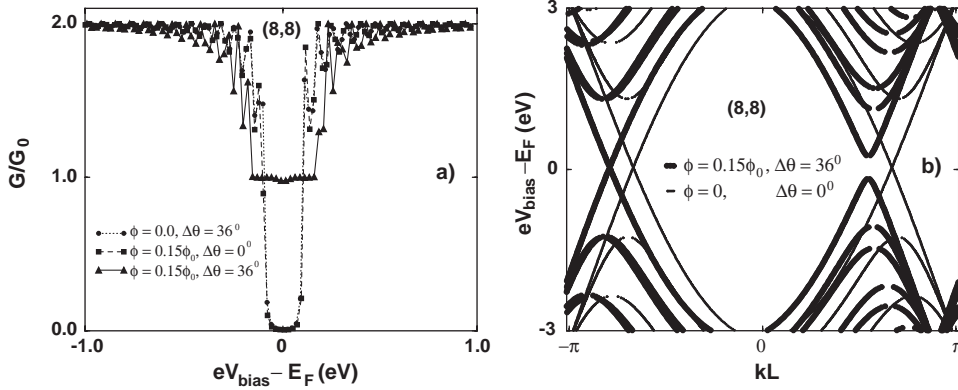


Fig. 3 – (a) Differential conductance of an (8,8) carbon nanotube subject to a $\Delta\theta = 36^\circ$ twiston extending over 100 unit cells and/or a magnetic flux $\Phi = 0.15\Phi_0$ in the axial direction. Both the twiston and the flux alone open up near-identical conductance gaps. A careful combination of nonzero flux and twist reopens a single conductance channel at small bias voltages. (b) Corresponding band structure of an infinite (8,8) carbon nanotube. Results for a straight tube in zero field are compared to those for a tube subject to an infinitely long uniform twist of $d\theta/dl = 0.36^\circ$ per unit cell and a magnetic flux $\Phi = 0.15\Phi_0$ in the axial direction.

These results, when combined, clearly demonstrate that finite twistons yield nonlinear I - V characteristics.

It must be stressed that the degree of twist required to open a pseudo-gap is small. For example in the finite (10,10) carbon nanotube of fig. 2(a), $\Delta\theta = 20^\circ$ over 100 unit cells is equivalent to $d\theta/dl \lesssim 1^\circ/\text{nm}$ only. The resulting perturbation to the Hamiltonian is therefore well within the limits of our model, where the twist is viewed as a frozen-in defect to the nanotube at low temperatures [23].

In a reasoning based on London theory, we now consider the effect of a uniform magnetic field on transport in straight and twisted nanotubes. Axially applied magnetic fields produce an Aharonov-Bohm effect in carbon nanotubes [16,17,28], which in the clean limit arises from the opening and closing of a band gap at the Fermi level. In the presence of a twiston, we now demonstrate that the reverse effect can occur, namely that an axial magnetic field can remove the twiston-induced conductance gap, resulting in a positive magneto-conductance. The effect of a combined structural twist and magnetic field on the conductance of nanotubes is discussed in fig. 3(a). These results show that a magnetic field may restore the zero-bias conductance of twisted armchair nanotubes from an essentially vanishing value to near half of the initial zero-twist value.

To understand this behaviour, we consider the roll-up process of a graphene sheet, spanned by the Bravais lattice vectors \mathbf{a}_1 and \mathbf{a}_2 , to an armchair nanotube. Structural twist of the tube, depicted in the inset of fig. 1(a), is related to a shear distortion of the initial graphene sheet. Let us assume that the electronic structure near E_F can be attributed to the nearest-neighbour $pp\pi$ interactions. The imposed structural twist is modeled by changing the relative strength of the hopping integral γ_i along the neighbour vector \mathbf{r}_i with respect to the undistorted reference value $\gamma_0 = 1$. Taking into account the diatomic basis of the distorted graphene sheet, we obtain a half-filled band with particle-hole symmetry and an energy gap between the valence and conduction band of

$$\Delta(\mathbf{k}) = |1 + \gamma_1 e^{i\mathbf{k}\cdot\mathbf{a}_1} + \gamma_2 e^{i\mathbf{k}\cdot\mathbf{a}_2}|.$$

During the initial roll-up process to an (n, n) nanotube, the two-dimensional electron momentum space of the graphene sheet collapses into a one-dimensional space with \mathbf{k} along the tube axis. Exposing the tube to a magnetic field adds the term $e\mathbf{A}/\hbar$ to \mathbf{k} , where \mathbf{A} is the vector potential, thus introducing a new phase factor [17]. Further noting that $\mathbf{k} \cdot \mathbf{a}_i = \mathbf{k} \cdot \mathbf{r}_i$, we find that the energy gap between the highest valence and lowest conduction band of a twisted tube becomes

$$\Delta(\mathbf{k}) = |1 + \gamma_1 e^{i\mathbf{k} \cdot \mathbf{r}_1} e^{i\phi} + \gamma_2 e^{i\mathbf{k} \cdot \mathbf{r}_2} e^{i\phi}|. \quad (1)$$

The phase $\phi = 2\pi\Phi/\Phi_0$ depends on the ratio between the magnetic flux Φ trapped in the tube and the fundamental unit of flux $\Phi_0 = h/e$. Note that the fundamental unit of flux used in this paper is twice the flux quantum, $\Phi_0 = h/2e$. The fundamental gap $\Delta = \Delta(\mathbf{k}_0)$, occurring at \mathbf{k}_0 , is the minimum value found in the Brillouin zone. We also note that $\Delta = 0$ for an undistorted tube in zero field.

In view of the twisted-tube morphology defined in fig. 1(a), it is convenient to introduce the quantity $\alpha = \mathbf{k} \cdot \mathbf{r}_1 = -\mathbf{k} \cdot \mathbf{r}_2$. From eq. (1) we find that $\Delta(\mathbf{k}) = 0$ only if $(\sin \phi / \sin \alpha) = (\gamma_1 - \gamma_2)$ and $(\cos \phi / \cos \alpha) = (-\gamma_1 - \gamma_2)$. Combining these equations, we find that the fundamental gap closes if

$$\cos 2\phi = \frac{(\gamma_1^2 + \gamma_2^2) - (\gamma_1^2 - \gamma_2^2)^2}{2\gamma_1\gamma_2} \quad (2)$$

and

$$\cos 2\alpha = \frac{1 - \gamma_1^2 - \gamma_2^2}{2\gamma_1\gamma_2}. \quad (3)$$

In other words, according to eq. (2), the twist-induced fundamental gap closes again, once the (n, n) nanotube is exposed to a magnetic field B

$$B = B_c \arccos \left(\frac{(\gamma_1^2 + \gamma_2^2) - (\gamma_1^2 - \gamma_2^2)^2}{2\gamma_1\gamma_2} \right) \quad (4)$$

along its axis, where $B_c = 2.28 \times 10^4 \text{ T}/n^2$. According to eq. (3), the longitudinal wave vector \mathbf{k}_0 , at which the fundamental gap vanishes, must satisfy the condition

$$\mathbf{k}_0 \cdot \mathbf{r}_1 = \frac{1}{2} \arccos \left(\frac{1 - \gamma_1^2 - \gamma_2^2}{2\gamma_1\gamma_2} \right). \quad (5)$$

The above heuristic model also demonstrates why the exact result of fig. 3(a) yields $G \approx G_0$ for the zero-bias conductance in the presence of a nonzero twist and flux, rather than the value $G = 2G_0$ for a twist-free tube in zero field. In the latter case, the two open scattering channels at E_F correspond to values of α (or wave vector \mathbf{k}) of opposite sign. For a given nonzero flux Φ and a corresponding sign of the phase ϕ , $(\sin \phi / \sin \alpha) = (\gamma_1 - \gamma_2)$ can be satisfied by only one of these channels. This is shown in fig. 3(b), where the dispersion curves in the presence of a compensating twist and flux are compared to those of a perfectly straight nanotube in zero field. As expected, reversing the sign of the twist angle switches the allowed conduction channel. Figure 3(b) also illustrates that the longitudinal Fermi wave vector \mathbf{k}_0 , which marks the band crossing at E_F , is shifted from the value for the unperturbed tube, as predicted by eq. (5).

In summary, we have analyzed for the first time the scattering properties of finite-size twistons and shown that these introduce nonlinear I - V characteristics associated with the opening of a pseudo-gap at E_F , thus effectively quenching the nanotube conductance. This conductance gap can be closed in an axial magnetic field, leading to a giant positive magneto-conductance. At small bias voltages, the conductance of a twisted tube in nonzero field can reach up to half the ballistic conductance value of a straight tube in zero field.

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