Universal number of conducting channels in doped carbon nanotubes

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Carbon nanotubes can be manufactured with a specific diameter but not with specific chiral vector, or conductance properties. A shift of the chemical potential can alter their conductance. Here we point out the possibility of obtaining a universal number of conducting channels for all same-radius tubes, regardless of their chirality, by a certain global shift of the chemical potential.

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The remarkable one dimensional properties of carbon nanotubes¹ renders them prime candidates for many applications in nanoelectronics. Having been manufactured with controlled radii, position and orientation, a crucial obstacle remains the inability to grow tubes with a known chirality, which determines whether the tube is metallic or semiconducting. Very recently, a novel method based on dielectrophoresis² demonstrated that metallic tubes can be extracted from a nanotube soot with very high enrichment. An alternative way of obtaining metallic tubes is by changing the chemical potential of existing tubes, which can be achieved, for example, by doping via simple exposure to air.^{3,4}

With a shifted chemical potential, semiconducting tubes may turn conducting,³ and metallic tubes may increase their number of conducting channels.⁴ Suppose we have an ensemble of tubes, metallic and semiconducting, with a similar radius; is there an amount of doping that will give the same number of conducting channels to all the tubes in the ensemble? In this communication we give a positive answer to this question, and show that this number is robust to some of the typical perturbations occurring in a nanotube.

A single wall carbon nanotube (SWNT) is a tubular graphite sheet, classified by two integers (n,m) which determine its radius and skew angle α ($0 \le \alpha \le 30^{\circ}$). The energy spectrum of SWNT is a laterally quantized spectrum of a graphite sheet, which has two inequivalent Fermi points, and, in their proximity, linear and isotropic spectrum

$$E = 3ta_{cc}\Delta k/2, \tag{1}$$

where t is the π -orbital transfer integral and a_{cc} the bond length.

If \hat{c} is a unit vector along the circumferential coordinate, the quantization lines lie at $\mathbf{k} \cdot \hat{c} = p/R$, where p are integers, and the six Fermi points lie at $\mathbf{k}_F \cdot \hat{c} = \pm (2n+m)/3R, \pm (n+2m)/3R, \pm (n-m)/3R$. If n-m=3q, where q is an integer, the Fermi points lie on quantization lines, and the tube is called primary-metallic; otherwise, when $n-m=3q\pm 1$, the tubes are semiconducting. Thus, the Fermi points of semiconducting tubes lie at $\mathbf{k}_F \cdot \hat{c} = \pm (3l\pm 1)/3R$, where l are three different integers. Hence, the shortest distance of the Fermi points to the nearest quantization lines is $\Delta k = |(\mathbf{k}_F - \mathbf{k}) \cdot \hat{c}| = 1/3R$, which is chirality independent. The strength of the semiconducting tubes is then $E_g = ta_{cc}/R$.

A small shift $|\Delta\mu|$ in the chemical potential, transforms the Fermi points to circles with radii of $2|\Delta\mu|/(3ta_{cc})$ (in the region of linear spectrum, as discussed below); consequently, the number of conducting channels is the number of quantization lines crossed by these circles (see Fig. 1). Primary metallic tubes open additional two channels, per Fermi point, at integer multiplets of the lateral quantization energy $E_R = 3ta_{cc}/2R$; the semiconducting tubes, having their highest occupied energy in the undoped state at a $E_R/3$ below the Fermi point, open a new channel at $|\Delta\mu| = (\nu + j/3)E_R$, where $\nu = 0,1,2,3,\ldots$ and j=1 or 2. Consequently, the total number of channels for a metallic tube, N_m , and the semiconducting, N_s , is

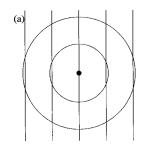
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$$N_{m} = 2\left(1 + 2\operatorname{Int}\left[\frac{|\Delta\mu|}{E_{R}}\right]\right),$$

$$N_{s} = 2\left(\operatorname{Int}\left[\frac{2}{3} + \frac{|\Delta\mu|}{E_{R}}\right] + \operatorname{Int}\left[\frac{1}{3} + \frac{|\Delta\mu|}{E_{R}}\right]\right),$$
(2)

where Int is the integer part, and the factor of 2 is due to the two Fermi points of SWNT. Figure 2 displays the total number of channels, which for all tubes coincides in the doping windows

$$-\frac{1}{6} < \frac{|\Delta \mu|}{E_R} - \frac{N}{4} < \frac{1}{6},\tag{3}$$



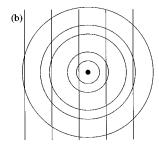


FIG. 1. Fermi circles at new conducting steps. **a**, Doping transforms the Fermi point (black dot) into a circle of increasing radius; the number of channels is the number of quantization lines crossed by the circle; each new step adds two channels (per Fermi point) for primary-metallic tubes. **b**, As in **a** but for semiconducting tubes. The Fermi point is at a distance $\Delta k = 1/3R$ from a quantization line. The number of channels increases here in steps of one.

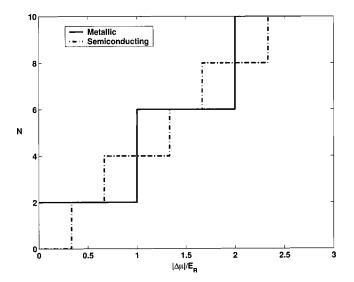


FIG. 2. Total number of channels (with two Fermi points) vs the absolute shift in the chemical potential $|\Delta\mu|/E_R$. The "doping windows" correspond to the ranges of $|\Delta\mu|/E_R$ where the number of channels of metallic and semiconducting tubes coincides [also given by Eq. (3)]. Effects of curvature and re-hybridization open small gaps near the conducting steps of primary metallic tubes. These gaps however fall outside the doping windows.

where $N=2,6,10,\ldots$ is the universal number of channels. Equation (3) gives the required doping window to obtain the same number of channels for same-radius tubes. We assumed linear spectrum of the π -orbital band-structure of a graphite sheet; for the linear approximation to hold, we require $|\Delta\mu| \ll t$; taking $|\Delta\mu| \sim NE_R/4$, gives $N \ll 8R/3a_{cc}$.

We should point out that it is the number of conducting channels, N, and the conductivity which are universal, not necessarily the conductance. The conductance is universal only in the limit of ballistic transport where $G = 2Ne^2/h$. If, on the other hand, tunneling to the tube is considered, the total conductance depends on the one-dimensional density-of-states (DOS), which is very different at the bottom of the doping windows for primary-metallic and semiconducting

tubes, for the following reason; as the two Fermi circles expand and touch new quantization lines, the new channel's dispersion-relation along the axis is purely parabolic, with a van Hove singularity of the DOS. Consequently, tunneling in/out of the tube at that filling is critically different than at a higher filling (still with the same number of channels). Since each doping window starts with two new channels for the semiconducting tubes, their DOS at that point will be markedly different from the primary-metallic one. This difference however vanishes as the doping increases. In the first doping window, for example the ratio of the Fermi velocities of semiconducting to metallic tubes is $\sqrt{1-(E_R/3\Delta\mu)^2}$.

Therefore, if the conductance is dominated by tunneling, it is not universal at the bottom of the window, despite of having a universal number of channels, while at the end of this range, universal conductance is regained without the need to assume perfectly transmitting ends.^{5–7}

Another complication may arise due to the nanotube's small curvature. The curvature causes two effects; first, $t_{\perp} \neq t_{\parallel}$, i.e., the lateral and longitudinal $(\pi - \pi)$ transfer integrals differ; secondly, π and σ orbitals mix. As a result, the π band-structure we used is perturbed, yielding (in both cases) a shift of the Fermi point away from a quantization line by a distance $\Delta k \propto \sin 3\alpha/R^2$; this gives rise to small energy gaps $^{8-10,12}$ $E_g^{\text{curvature}} = 3ta_{cc}^2 \sin 3\alpha/16R^2$ in otherwise metallic tubes; these gaps were experimentally observed. The above mentioned energy gaps do not, however, affect the universality window (see Fig. 2) since $E_g^{\text{curvature}} \ll E_g$ for practically all tubes. The constant of the property of the practically all tubes.

In conclusion, we specified the ranges by which the chemical potential should shift for all same-radius tubes to have the same number of conducting channels, regardless of their chiral angle. We showed that this number is unaffected by effects of small curvature and re-hybridization of the π and σ orbitals.

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