Transport through higher subbands of a carbon nanotube

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Abstract

The sub-band spacing can be comparable to the bias and kT in large diameter carbon nanotubes. As a result, the role of higher sub-bands cannot be neglected in transport. We discuss two interesting effects involving single particle transport such nanotubes: (i) The transmission probability of electrons at the crossing bands (around E=0) and higher sub-bands are quantitatively different. As a result, we show that the small bias resistance may be larger when the Fermi energy is away from the band center as opposed to being close to the band center. (ii) The primary contribution to current flowing in the presence of an applied bias is due to the crossing sub-bands. This is a result of the electron in the higher sub-bands undergoing Bragg reflection. As a consequence, in an idealized case where scattering is neglected, the differential conductance cannot be much larger than $4e^2/h$.

Most experimental[1-3] and theoretical work of electron transport in individual nanotubes deal with single wall nanotubes (SWNT). In these experiments, the spacing between sub-bands is typically larger than the applied voltage and kT. Recent experiments on multi wall nanotubes (MWNT)[4-6] are fundamentally different in that the sub-band spacing is comparable to kT and the applied voltage. It is further believed that transport in these experiments primarily takes place along individual layers, with little inter-layer coupling. Two salient features in the work of Frank et. al[4] are: a peak in the bar chart of small bias conductance versus number of measurements around $2e^2/h$ and an anamolous increase in differential conductance with increase in applied voltage. The second feature refers to the point that the increase in differential conductance is much smaller than the value obtained by a picture that simply counts the increase in number of modes (or sub-bands) with increase in applied voltage. Motivated by these recent studies on MWNT, we study the role of higher sub-bands in transport with the aim of clarifying the simple single particle physics involved. This paper deals with two different issues involving transport through higher sub-bands: (i) the role of large reflection probability at higher sub-bands in comparison to the band center and (ii) the role of Bragg reflection. We emphasize that Bragg reflection plays a unique role in nanotube wires.

Most theoretical studies of nanotube conductance have so far calculated the phase coherent transmission coefficient. Schonenberger et. al,[5] have recently measured phase coherence lengths (L_ϕ) in MWNT that are as small as 100 $\AA$. As the phase coherence length plays an important role in determining the conductance, the first part of our discussion takes finite L_ϕ into account.

The two terminal resistance of a phase coherent sample can be written as,

$$\begin{aligned} R &= R_{contact} + R_{intrinsic} \\ &= \frac{h}{2e^2}\{\frac{1}{\sum_m \int f'(E)} + \frac{\int \sum_m R_m(E) f'(E)}{[\sum_m \int f'(E)] \cdot \int \sum_m T_m(E) f'(E)}\} , \end{aligned} \tag{1}$$

where, $f'(E) = -df(E)/dE$. $R_{contact}$ is resistance due to the nanotube-contact interface (which has assumed to be perfect) and $R_{intrinsic}$ is the intrinsic resistance of the nanotube

sample due to scattering from defects. m is the sub-band index, $T_m(E) = \sum_n T_{mn}(E)$ is the two terminal transmission probability and $R_m(E) = 1 - T_m(E)$ is the reflection probability.[7] In the event that all channels are perfectly ballistic, the two terminal resistance is equal to the contact resistance. In the case of a nanotube with length (L) larger than L_ϕ, Eq. (1) is not valid. The essential physics can however be captured by the following phenomenological modification.[7] Let the phase coherent transmission coefficient of a L_ϕ long nanotube section be represented by $T_m^\phi(E)$. Then, the resistance can be thought of as having a contribution due to the contacts $\frac{h}{2e^2}\frac{1}{\sum_m \int f'(E)}$ [which is not different from the phase coherent case; Eq. (1)] and L/L_ϕ additional contributions due to the L_ϕ long sections:

$$R \sim \frac{h}{2e^2}\{\frac{1}{\sum_m \int f'(E)} + \frac{L}{L_\phi} \cdot \frac{\int \sum_m R_m^\phi(E) f'(E)}{[\sum_m \int f'(E)] \cdot \int \sum_m T_m^\phi(E) f'(E)}\}. \tag{2}$$

The important point of Eq. (2) is that the intrinsic resistance depends on two ratios,

$$\frac{L}{L_\phi} \text{ and } \alpha = \frac{\int \sum_m R_m^\phi(E) f'(E)}{M \int \sum_m T_m^\phi(E) f'(E)}, \tag{3}$$

where $M = \sum_m \int f'(E)$ is the number of sub-bands involved in transport around the Fermi energy. For simplicity, we assume that the reflection probability of all sub-bands (R_m) at a particular energy are similar, $\int R_m^\phi(E) f'(E) = r$. Then α has a particularly intuitive and simple form:

$$\alpha = \frac{1}{M} \cdot \frac{r}{1-r} = \frac{r}{Mt} \tag{4}$$

i.e., α is the ratio of the reflection probability and the number of sub-bands times the transmission probability. If $\frac{L}{L_\phi}$ is much larger than $\alpha^{-1} = \frac{Mt}{r}$, the contribution of the second term (intrinsic resistance) to the total resistance [Eq. (1)] can be non trivial and the an interesting scenario develops where the four terminal reistance can be larger when many sub-bands (as opposed to only the crossing sub-bands) are involved in transport (discussion in the next two paragraphs).

The above discussion is very relevant to nanotubes because of the values r and M assume at different energies. As energy increases from the band center, both the number of sub-bands M and the reflection probability increase. Provided that the reflection probability

increases fast enough, the value of $\alpha = \frac{Mt}{r}$ can be *smaller* at higher energies than at the band center. The consequence of this is explained using a concrete calculation below.

We calculate r in the context of uniform disorder as in Ref. 8. The transmission probability of a 100 $\mathring{A}$ long $(40, 40)$ nanotube region with disorder is plotted in Fig. 1. The energy of the first sub-band opening for this tube is approximately at 0.25eV and this energy decreases with increase in tube diameter (it is 0.15eV for a (60,60) nanotube). The important point to note in Fig. 1 is that the reflection probability increases as sub-bands are added. There are 2, 6, 10 and 14 sub-bands at energies of 0, 0.3, 0.7 and 1.0eV respectively, and the corresponding values of α for the dashed line are xxx. So the intrinsic resistance as measured in a four terminal setup (total resistance minus contact resistance) *increases* with increase in number of sub-bands! That is, in an experiment measuring the small bias conductance as a function of the Fermi energy through the sample: the resistance will be larger when the Fermi energy is located at an energy where there are many sub-bands, in comparison to the case when the Fermi energy is located at the band center. Fig. 1 considered the change in transmission in the case of defects that correspond to changing the on-site potential of the carbon atoms.[8] Our observations however do not rely on the detailed model of defects. Kortryko et. al have shown that energies around E=0 corresponding to the crossing sub-bands are least affected compared to higher sub-bands using other defect models, and Ando et. al have come to similar conclusions using analytical methods that do not assume specific defect models. We should mention that the discussion above has assumed that L_ϕ in the nanotube is not very sensitive to the location of the Fermi energy / number of sub-bands.

The discussion so far has centered on the case where the potential drop across the nanotube is insignificant (small bias case). We now discuss the second aspect of this paper, which concerns the differential conductance versus applied bias in the case of a defect-free nanotube with good contacts to the voltage source. We calculate the current versus applied voltage when the voltage drops linearly across the nanotube. The motivation for this

stems from the fact that a number of authors have reported calculations of reasonably large screening lengths even for armchair tubes. The central point of this study is that an applied bias across the nanotube results in a *transport bottle neck*, which will result in a smaller than expected increase in differential conductance versus applied bias in the experiments of Ref. 4. This point is best understood by presenting results of an I-V calculation. We consider the current versus voltage in a 1000 $\AA$ long (10,10) nanotube by assuming an almost linear drop in applied bias. Perfect carbon nanotube leads are assumed and the current is computed using the procedure in reference 8. Fig. 3 is the calculated I-V curve. The surprising feature here is that the maximum conductance and current are only $4e^2/h$ and xxx respectively. That is, the conductance is equal to the value that one would get if only two modes conduct. What happens to the contribution of the other modes injected into the nanotube? The answer to this lies in Fig. 3, which is a plot of the $E(k)$ relationship of a nanotube at different positions along the length of a nanotube. The band centers are at V_a (the applied voltage) and zero at the left and right ends of the nanotube respectively. Close to the left contact, electrons injected at the band center in the two available modes flow to the right contact unimpeded. This is however not the case for higher sub-bands. The k-vector of an electron injected from the left contact into a higher sub-band increases and eventually corresponds to the value at its sub-band extrema, where Bragg reflection occurs. The solid horizontal line is an example of an electron injected from the left at a higher sub-band, which undergoes Bragg reflection at the location of the arrow. Such a reflection occurs for all other (non-crossing) sub-bands too. This explains the maximum conductance of $\frac{4e^2}{h}$ in Fig. 2(b) and the reason for zero current contribution of the non-crossing sub-bands. It should be noted that in Fig. 2(a) the current plateaus out, which implies the zero differential conductance in Fig. 2(b). Again, this can be understood by using Fig. 3. Applying a larger than about 3.1 V[10] leads to some energy ranges in the crossing bands being Bragg reflected, while new energy ranges in the crossing bands contributing to transport. They conspire in a manner so as to keep the total current constant in the voltage range shown.[?] As we are not aware of any MWNT nanotube experiments with such a large applied voltage (the

nanotubes typically burn out), we would like to stress the smaller applied voltages, where electrons are still injected into many sub-bands.

Some remarks regarding the relationship of the above calculations to experiments are necessary. Nanotube experiments typically involve scenarios (a) where both contacts are well coupled to the nanotube or (b) one or both contacts are poorly coupled to the nanotube. The results of Fig. 2 correspond to both contacts being well coupled to the nanotube. If on the other hand one contact was poorly coupled to the nanotube such that a major fraction of the applied voltage dropped prior the nanotube, then electrons injected at higher sub-bands may be transmitted to the right contact. As a result the differential conductance may increase with applied voltage. The conductance contribution due to energies close to the band center will however be much smaller than $\frac{4e^2}{h}$ due to the large contact resistance. Two other physical mechanisms that lead to differential conductances larger than that shown in Fig. 2(b) are discussed: (a) We assumed a rather linear drop in the applied voltage. If most of the applied voltage dropped across short lengths of the tube such that the electric field is large, sub-band to sub-band tunneling will aid in leading to larger differential conductances. (b) An electron traveling in a higher sub-band can can loose or gain energy via scattering, which can result in a wave vector change that will aid the electron to reach the right contact.

The purpose of this paper is to present aspects involved in electron transport through higher sub-bands of a carbon nanotube. The first effect we discuss concerns the role of the competition between increase in number of sub-bands (Mt) and increase in reflection probability (r)in determining the conductance. We show that the small bias resistance may be larger when the Fermi energy is at an energy where many sub-bands are present as opposed to the case where the Fermi energy is close to the band center. The second effect discussed in this paper concerns the role of Bragg reflection in an experiment involving current versus applied voltage. We showed that as a result of the unique band structure of carbon nanotubes, Bragg reflection is an important mechanism for reduction of differential conductance. These effects will be important in large diameter MWNTs, where the higher sub-bands are easily accessible in transport experiments. Some drawbacks, which are beyond

the scope of the present work have been discussed in the previous paragraph.

I am grateful to Zhen Yao and Cees Dekker for many discussions on SWNT transport experiments. During NANOTUBE-99, I have also benifited from discusssions with Adrian Batchold and Walt de Heer. The results of this paper, however, in no way means implies their concurrence on the subject matter. I would also like to acknowledge T. R. Govindan for useful discussions on some computational aspects.

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[10] The voltage corresponds to the hopping parameter which was chosen to be 3.1 eV, which is the energy at which the various bands meet.

[11] The reason for this can be easily analysed by neglecting all higher sub-bands and applying larger applied biases in Fig. 3. Such a picture was presented in Molecular Electronics, Sci-

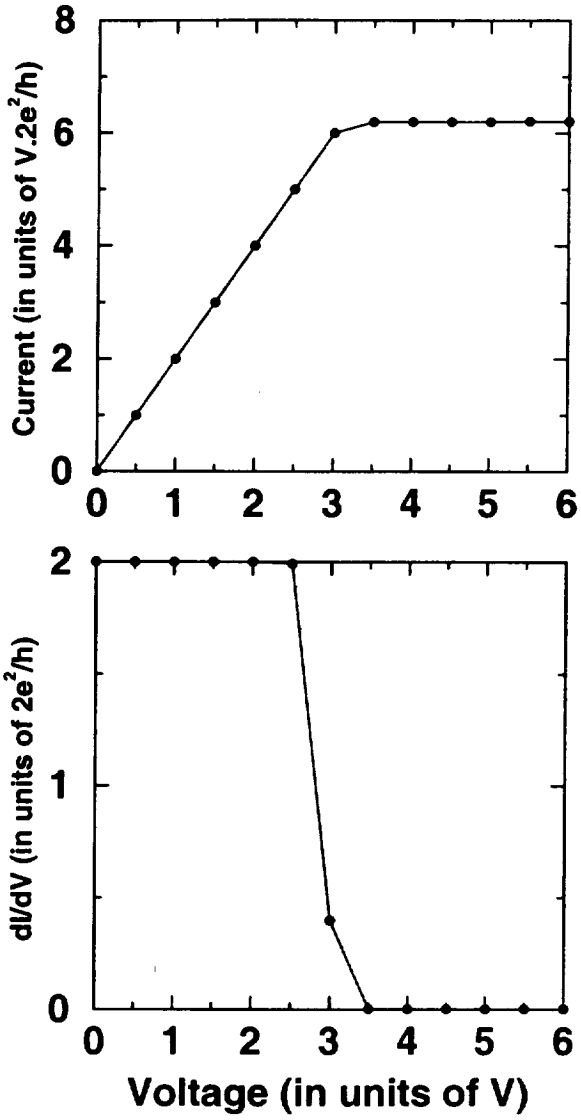
ence and Technology, PR, USA, December 1997. Please see *http* : *//www.nas.nasa.gov/* ~ *anant/PRtalkIV* for a detailed explanation.

Figure Captions:

Fig. 1: The transmission versus energy for a 100 $\mathring{A}$ long (40,40) armchair tube. The three curves correspond to two no defects and two different strengths for defect scattering.

Fig. 2: (a) The current versus voltage curve of a (10,10) nanotube with uniform voltage drop across its length. The length was taken to be 1000 $\mathring{A}$. (b) The important feature is that inspite of the large number of modes at higher energies, the maximum differential conductance is $4e^2/h$.

Fig. 3: E(k) relationship at different sections along the length of a nanotube. Each rectangular box represents an energy versus wave vector diagram with the band bottom equal to the electrostatic potential at that section. This figure aids in understanding the results shown in Fig. 2: The crossing bands carry current to the right contact but all other bands are reflected to the left contact because its wave vector reaches a point where the velocity $dE/dk = 0$ (Bragg reflection).


Current (in units of V.2e²/h)
8
6
4
2
0
0 1 2 3 4 5 6
dI/dV (in units of 2e²/h)
2
1
0
0 1 2 3 4 5 6
Voltage (in units of V)

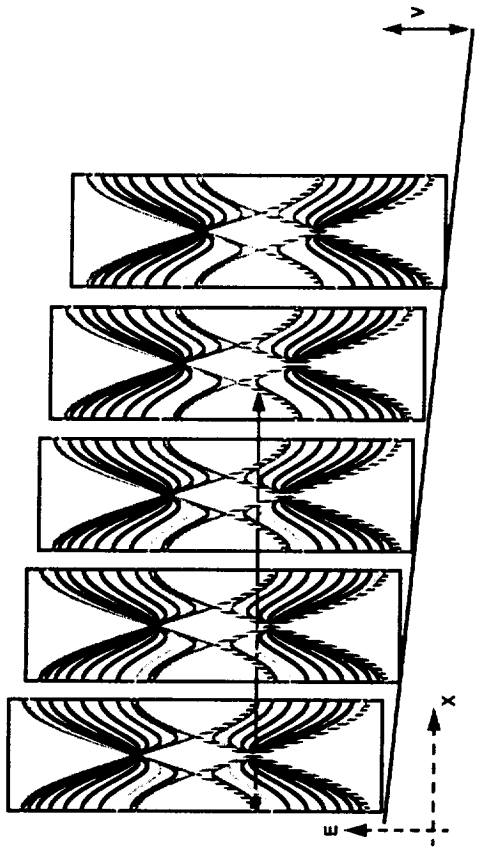
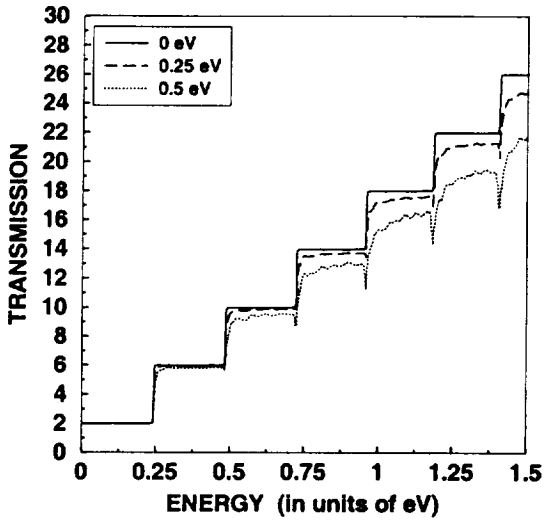


Fig. 3 / Anantram

FIGURES



Anantram / Fig1