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Quantum Transport Calculations of Carbon Nanobube Based Materials

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1. Introduction

Carbon nanotubes (CNTs) are fascinating low dimensional objects that offer a challenging playground to deepen the analysis of quantum phenomena at the nanoscale. Electronic transport is in this context of particular concern. Single-walled metallic CNT are long ballistic conductors owing to the vanishing contribution of backscattering from elastic disorder. Within the Fermi Golden Rule, whatever the scattering mechanism, the estimated elastic mean free paths usually reach several micrometers provided that the Fermi level is located close enough to the charge neutrality point. This property has been evidenced experimentally by measuring the conductance of small diameter metallic tubes contacted to palladium electrodes. Ballistic CNT-FET have been also fabricated with semiconducting CNT.

Electron-phonon coupling in CNT has been intensively investigated theoretically in relation with temperature-dependent resistivity in metallic CNTs. One of the important consequence of e-ph scattering is to restrict ballistic transport to the low bias regime, for which propagating electrons can only be coupled to low-energy acoustic phonon modes. In this regime the experimental temperature dependence of the tube resistance is linear, and driven by acoustic phonon modes. The increase of the applied bias potential across the CNT further promotes the contribution of higher energy (optic) modes which more significantly impact on the tube conduction, resulting in a saturation regime, or a decrease, of the current versus potential depending on the thermalization rate.

In this presentation, we focus on quantum transport through CNTs in the presence of elastic disorder and e-ph interaction. We will extensively use the time-dependent wave-packet technique which is a real space (order N) computational framework to study the dynamical properties of quantum wave-packets, as well as the corresponding conductance scaling behaviors, within the framework of the Kubo linear response.

We will focus on the modelling approaches to tackle with time-dependent one-body description of electronic motion in the presence of lattice vibrations. A scheme to solve the associated time-dependent Schrodinger equation as well as quantum transport in the Kubo framework will be presented. The calculated temperature dependence and length scaling of the resistance will be shown to well agree with experimental results.

2. Time-Dependent Wave-Packet Diffusion Approach

The general electronic transport theory in the response regime based on the Kubo formula for the dc-conductivity is relied on the measure of autocorrelation average of wave packets velocity operators. Time-dependent diffusion coefficient is defined as

$$D(E_F,t)=\frac{1}{2t}\frac{Tr\left[\delta(E_F-\hat{H})\left(\hat{U}^{+}(t)\hat{x}\hat{U}(t)-\hat{x}\right)^2\right]}{Tr\left[\delta\left(E_F-\hat{H}\right)\right]} \qquad (1)$$

where x is the electron position operator along the tube axis. $D(E_F)$ represents the diffusion coefficient at the Fermi energy where $D(E_F,t)$ takes the maximum value. Operator U(t) represents the time-evolution operator and is broken up into small increments of duration $\triangle t$ so that the variation of the Hamiltonian operator becomes small,

$$\hat{U}(t)=\prod_{n=0}^{t/\Delta t-1}\left[\sum_{n=0}^{\infty}e^{-i a\Delta t/\hbar}h_n i^n J_n\left(-\frac{b\Delta t}{\hbar}\right)T_n\left(\frac{\hat{H}(t)-a}{b}\right)\right] \qquad (2)$$

Here, the energy spectrum of H(t) has the interval [a-b, a+b], $h_0=1$, and $h_n=2$ (n > 1) . T_n is the Chebyshev polynomials and J_n represents the Bessel function. From the obtained diffusion coefficient $D(E_F)$, the one-dimensional resistivity ρ defined by the resistance per unit length, the mean free path ℓ_{mfp}, and the relaxation time τ are computed [1-4].

3. CNT Transport Properties

3.1 Channel-length dependence of CNT resistance –from diffusive to ballistic regimes-

To take the realistic phonon-vibration effects on the transport properties into account, we use the phonon modes obtained from the molecular dynamics simulation and study the transport properties of the impurity-free (5,5)-CNTs at the room temperature (300 K). In the diffusive regime, the time-dependent diffusion coefficient D(E,t) of CNT with 7.5 μ length saturates to $D(E_F)=220$ nm^2/fs due to electron-phonon scatterings. We obtain the resistivity ρ = 12 k Ω/μ m, the mean free path ℓ_{mfp} = 537 nm, and the relaxation time τ = 654 fs. We note that the estimated and also experimentally observed mean free path changes from 300 nm to 1.6 μ m at low bias regime.

In the ballistic regime without any scatterings, the time dependent behavior of the diffusion coefficient D(E,t) increases monotonically. The slope is equal to $v_F^2 t/2$, since the square length of the wave packet, $< (x(t)-x(0))^2 >_{EF}$, is given by $v_F t^2$ when electrons pass through the nanotube at the Fermi velocity. D(E,t) takes the maximum value at time $t = L/v_F$ and so the diffusion coefficient D(E_F) is proportional to the nanotube length as given by $L v_F /2$.
Using $\rho = R/L = (h/2e^2)(v_F/4/D(E_F))$, we obtain the length independent resistance as $(2G_0)^{-1}$, which corresponds to the inverse of the two conductive channels at the Fermi energy and is consistent with ballistic transport character in Landauer formula. Here, G_0 is defined by $2e^2/h = (12.9 k\Omega)^{-1}$.

Next, we consider the length dependence of the resistance. The bold curve in Fig.1 shows the resistance as a function of length. We see that the resistance is equal to the $6.45\ k\Omega = (2G_0)^{-1}$ when the length is short. On the other hand, when the length is much longer than the mean free path, electrons are scattered many times by phonons, changing the transport properties into a diffusive character.

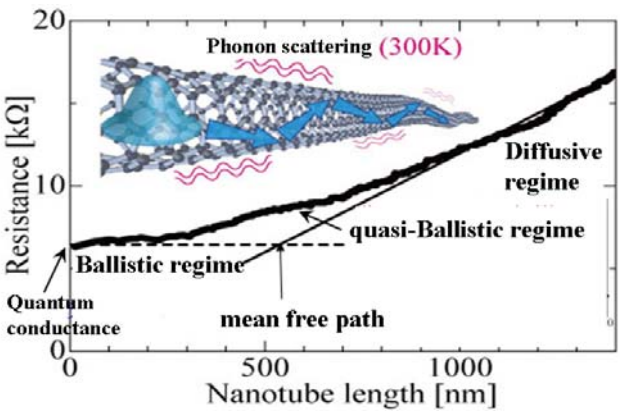

Fig.1 Chanel-length dependence of the resistance of (5,5) carbon nanotubes with room temperature (T=300K).

In this diffusive regime, the resistance is linearly proportional to the length (Ohm's law) as shown in Fig.1. The straight broken line in Fig.1 represents the ballistic limit of resistance $(2G\_0)^{-1}$, while the straight thin line represents the diffusive transport limit. The intersection point of these lines corresponds to the mean free path. It should be noted that the resistance deviates from these lines around the mean free path. We note that this behavior is fully consistent with experimental data [5].

3.2 Temperature dependence of CNT resistance

Here, we present the calculated results on the temperature dependence of the resistivity. Figure 2 shows the one dimensional resistivity of the (5,5)-CNT as a function of several temperatures in the diffusive transport limit with the nanotube length of 7.5 μ m. The resistivity shows linear dependence on the temperature, which is in good agreement qualitatively with experimental observations [5] and other theoretical calculations.

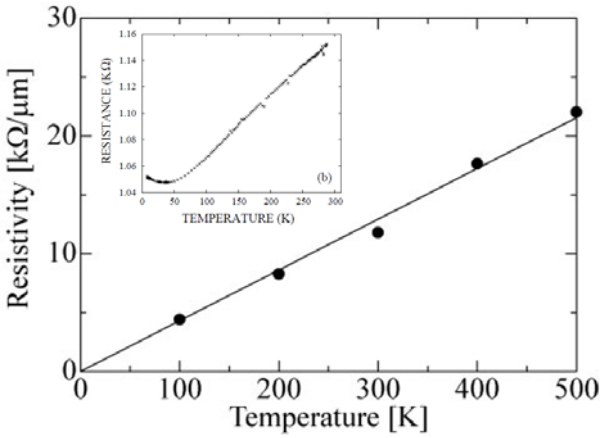

Fig.2 Temperature dependence of the resistance of (5,5) carbon nanotubes in the diffusive regime with the length of 7.5 μ m.

4. Conclusions

We have presented an efficient time-dependent wave packet diffusion method based on the Kubo formula allowing the exploration of scattering phenomena in CNT in presence of both elastic and dynamical disorders. This method has been shown to provide numerical results in very good agreement with both analytical derivation as well as experimental measurements. Therefore, given its efficient predictability efficiency, its applicability to other complex form of carbon based materials and devices is thus very promising for both material science and advanced nanotechnology.

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