Low-T Quantum Transport in Carbon Nanotubes: Role of Vacuum Fluctuations in Loss of Phase Coherence

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ABSTRACT

The process of environmental decoherence is seen to occur when we include the quantum dynamics of a system and its environment: the innovative idea is that environmental degrees of freedom are relevant even though the coupling to them is only weak. The effect of vacuum fluctuations on electron coherence is known: the time-varying electro-magnetic field produces a time-varying Aharonov-Bohm phase. But it is known too that a conducting boundary modifies the properties of the zero-point fluctuations which, introducing a random stress, affect the electronic transport properties in a carbon nanotube via interaction with a random potentials (impurities) long the tube. We shall discuss the situation in which a quantum-mechanical system, the ballistic electrons in nanotube, is disturbed not just by a classical system but another quantum-mechanical system, the vacuum fluctuations due to conducting boundary , about which there are statistical uncertainties.

Keywords: quantum transport, carbon nanotube, phase coherence,localization, vacuum fluctuation

1 INTRODUCTION

Among the main items in the design of new generation of electronic devices there are the measurement and understanding of the current-voltage response of an electronic circuit in which molecular systems like carbon nanotubes (CNTs) act as conducting elements. It is well known that environment-induced decoherence is omnipresent in the microscopic world so that the destruction of phase coherence due to coupling of a system to an irreversible bath [1-3] is a subject important because of its role in suppression of phenomena resulting from quantum interference effects such as Aharonov-Bohm interference, weak localization and universal conductance fluctuations. The study of quantum mechanical decoherence is a central problem in the physics of condensed matter systems coupled to an environment where, in the zero-temperature limit, the only source of decoherence are provided by vacuum fluctuations (Casimir effect). Using a phenomenological approach we have analyzed the effects of weak disorder (random deformation potential) induced by the vacuum fluctuations due to the presence of a conducting boundary, on the electronics transport properties of CNTs, in particular the destruction of ballistic conduction in metallic carbon nanotubes due to loss of phase coherence

2 CASIMIR FORCE ON CARBON NANOTUBE

The Casimir effect [4] is the force between two unchar-ged solid objects that arises from quantum fluctuations in the zero-point (vacuum) energy of the electromagnetic field [5]; Lifshitz described this force as the retarded electromagnetic interaction between macroscopic dielectric bodies characterized by some dielectric constant [6-7]: anyhow, the Casimir force is the most accessible effect of vacuum fluctuations in the macroscopic world and is strongly dependent on the shape of the bodies switching from attractive to repulsive in function of the size, geometry and topology of the boundaries.

Consider now a model in which a metallic cylinder of radius R and length L ($L >> R$) is assumed to be with its axis parallel to a flat conducting boundary at distance d. If $d << R$, the proximity (or Deriagin) approximation [8] (the approximation assumes that the force on a small area of one curved surface is due to locally “flat” portions on the other surface) can be applied to the case of the Casimir attraction; let also consider the case of small separations d such that $d << c/\omega_p$ where ω_p is the plasma frequency of the free electrons with density n and defined by [9]

$$\omega_p^2 = 4\pi \frac{ne^2}{m}$$

For small separations $d << 30nm$ we can use the Lifshitz formula (in [6] between two plates) for the force per unit area between cylinder and plate:

$$f(d) = \frac{-i\hbar}{8\pi^2 d^3} \int d\xi \frac{[\varepsilon(\xi) - 1]^2}{[\varepsilon(\xi) + 1]^2} \quad (1)$$

where ε is the dielectric permittivity, assumed to be the same for both cylinder and plate. The explicit form of ε in the Drude approximation is [9]

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} \qquad (2)$$

where τ is the momentum relaxation time and since τ^{-1} is much smaller than ω_p the corresponding term can be neglected when integrating Eq. (1). It follows from Eqs. (1) and (2) that in the case of a cylinder we have the force for unit length

$$F(d) = \frac{3\hbar\omega_p R^{1/2}}{256 d^{5/2}} \qquad (3)$$

In the case of the Casimir force on carbon nanotube near a conducting boundary, the effective stress on nanotube in proximity zone is

$$F_{eff} \approx \frac{4F(d)}{\pi R} = \frac{3\hbar\omega_p}{64\pi R^{1/2} d^{5/2}} \qquad (4)$$

being in this case the absolute value of the "squeezing" force $|F_{cylinder}| << F_{eff}$. The mechanical strain due to F_{eff} induce change in band structure of SWNT by changing d, the minimal distance between conducting boundary and nanotube.

3 QUANTUM TRANSPORT IN SWNT

Till now it remains not completely explained how mechanical deformation affects the intrinsic electrical properties of nanotubes, but in [10] it is reported an experimental and theoretical elucidation of the electro-mechanical characteristics of individual single-walled carbon nanotubes under local-probe manipulation: in situ electrical measurements have revealed that the conductance of a sample can be reduced by two orders of magnitude when deformed and simulations have indicate that this effect is owing to the formation of local bonds caused by the mechanical pushing action. In [11] Minot et al. show that the band structure of a carbon nanotube can be dramatically altered by mechanical strain.

3.1 Kubo Formula for Conductivity

For infinity systems, in terms of complex conductivity [12] $\sigma(\omega)$, we can write the linear response $\mathbf{J}(t)$ of a sample to an external electric field $\mathbf{E}_{loc}(t)$ as $\mathbf{J} = \sigma\mathbf{E}_{loc}$ where

$$\sigma(\omega) = \frac{ne^2\tau}{m}\frac{1}{1 - i\omega\tau} \qquad (5)$$

is the classical Drude conductivity (note that $\sigma(0)$ is the static conductivity). This is a simplified version of a more general formula for actual local current measured by experimentalists (generalized Ohm's law)

$$J_\alpha(\mathbf{r},t) = \int d\mathbf{r}' \sum_\beta \sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) E_\beta(\mathbf{r}',t) \qquad (6)$$

and the (non-local) conductivity $\sigma_{\alpha\beta}$ is response to actual (external + induced) electric field and is given by the Kubo formula [13] (where periodic boundary conditions and coupling of only the charge degrees of freedom, none spin degree of freedom is considered, to external $\mathbf{E}$-field are assumed)

$$\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = \frac{e^2}{\hbar\omega}\int_0^\infty dt e^{i\omega t}\left\langle \Psi \left| [j_\alpha^+(\mathbf{r},t), j_\beta(\mathbf{r}',0)] \right| \Psi \right\rangle + \\ + \frac{ne^2}{m\omega} i\delta_{\alpha\beta}\delta(\mathbf{r} - \mathbf{r}') \qquad (7)$$

The wave function Ψ is the ground state of the many-body Hamiltonian which contains all possible interactions in the solid (except the interaction between the total electric field and the particles of the system) and the first term in (7) is called retarded current-current correlation function. Kubo first derived the equations for electrical conductivity in the solid and Kubo formulas are the name applied to the correlation function which describes the linear response. But this procedure is physically incorrect as a way of defining the conductivity in a finite system (in which electrons enter from an external electrode at one end and are removed at the other).

3.2 Physics of Conduction Process in 1D Real System

In a finite (ideal) sample if the chemical potential is higher at one lead (electrons of the large reservoir with constant μ_1) than at the other lead (with constant μ_2) the current is the response to the gradient of chemical potential for electrons not to the electric field; in other words, if $\mu_1 > \mu_2$ and e is the absolute value of the electronic charge, the voltage difference ΔV between the two baths due to flow across the sample of the current I is

$$\Delta V = \frac{I}{G_c} = \frac{\mu_1 - \mu_2}{e} \qquad (8)$$

where

$$G_c = \frac{e^2}{\pi\hbar}T(E_f) \qquad (9)$$

is the irreducible conductance measured between the two outside reservoirs being T the transmission probability for channel (to go from electrode 1 to electrode 2). The inelastic processes (which break the time-reversal invariance and the phase coherence of the states at the two extremities, dissipate energy and restore equilibrium) in this case are assumed to exist only in the two electrons baths, so that the ramdomized phase of the injected and absorbed electrons through these processes results in no phase relation between particles. At low temperature the true conductance G due to barrier (including spin degeneracy) is correctly given by the transmission and reflection coefficients of the sample (in presence of only elastic scattering for the electrons at the Fermi surface with a linear series of random scatterers connecting the two reservoirs) by the Landauer , not the Kubo, formula [14]

$$G = \frac{e^2}{\pi\hbar}\frac{T(E_F)}{1-T(E_F)} \qquad (10)$$

Electronic transport measurements [15] on individual SWNT demonstrate that , in the absence of scattering (then the transmission probability is $T = 1$), the momentum relaxation length and the localization length are much larger than the wire length and the transport in these systems is ballistic[1]: the wavefunction of the electron is extended over the total length of the nanotube and there are only two channels which contribute to the electronic transport giving $G = 2G_c$. However, as already outlined, in presence of some mechanism of scattering the conductance is described by the Landauer formula (10) and the conductance is no longer exactly quantized.

Not only, in [16] Bockrath et al. observe a Luttinger-liquid behavior in (rope of) SWNT's in measurements of the electrical transport as a function of temperature resulting in a power laws for linear response conductance (in this case T is the temperature)

$$G(T) \propto T^{\alpha} \qquad (11)$$

where $\alpha = f(g)$ and $g = \left(1 + \frac{2U}{\Delta}\right)^{-1/2}$ (U is the charging energy of the tube and Δ is the single-particle level spacing).

1 The important length scales are the coherence length l_φ, the energy relaxation length l, the elastic mean free length l_0, the Fermi wave length λ_F of the electron, the atomic Bohr radius a_0 and the sample size L and in mesoscopic system $a_0 << \lambda_F \le l_0 < L < l_\varphi \le l$.

3.3 Weak Localization and Coherence Loss in SWNT

When the temperature is so high that the conductivity can be treated as local quantity, as in Anderson localization[2] which deals with wave function of the single electron in presence of random potential, the conductance is obtained by combination of smaller parts of materials; but when the temperature is low (or the sample is small) the dephasing length l_φ is greater than the sample linear dimensions L so that the quantum corrections to the conductivity are non-local and the conductance can no longer be treated as a self-averaging quantity. Since the lack of self-averaging of the conductance is a feature of mesoscopic conductors (where the electrons maintain their quantum-mechanical phase coherence) in SWNT it must be analyzed the effects of weak disorder (random deformation potentials here indicated as impurities) induced by the vacuum fluctuations due to the presence of some conducting boundary. Due to the existence of these impurities the transport is more diffusive than ballistic (the existence of scattering is possible in both regimes but in diffusive one we have that $l = v_F\tau << L$ so that the material is characterized by a relatively low mobility) though the elastic scattering of the electrons, if these impurities are equivalent to static defects, can modify the interference terms but does not cause decoherence [14]. At low temperature the conduction take place mainly with electrons at Fermi energy and, due to some gate potential, the Fermi point upon which the electrons travel can be shifted slightly, therefore it is possible that an electron that moved on one side (path) of an impurity begins to move on the other side (path) after the shift. This process (analogous to Aharonov-Bohm effect in the presence of some magnetic field) induced a quantum fluctuation of the conductance of the order of $2e^2/h$ and depends on the exact configuration of scattering centers within the sample: these two paths are time-reversed with respect to one another and since the electron return to its original position it can interfere with itself creating an additional resistance called weak localization.

From semiclassical point of view it is possible to calculate this additional resistance holding in the mind that the conductivity is related to the current-current correlation function, as in eq. (7), and being $D = v_F^2\tau$ the diffusion coefficient and $l_\varphi = \sqrt{D\tau_\varphi}$ for 1D we get [14]

2 The localization is, in the first instance, a property of the states in random quantum mechanical systems and can be interpreted by total back-reflection of particles from potential barriers so that they become loclized in a single potential well.

$$\square\square\square\ \square\frac{e^2}{\square\hbar} l_{\square}(1\square\sqrt{\frac{\square}{\square+\square_{\square}}}) \quad (12)$$

Mohanty and Webb [17] prove that zero-point fluctuations cause the dephasing in one dimensional quantum wire at low temperature (ascribed to finite broadening of Fermi surface) presenting a zero-point-limited dephasing time $\square_0$ in good agreement with the measured saturation values $\square_{\square}$ found in many experiments.

A more sophisticated theory tells to us that in presence of a vector potential, for $\square\square\square << 1$, the probability of return path in a disordered SWNT can be conveniently obtained by calculating the "Cooperon" $C_{\square}(\mathbf{r},\mathbf{r}')$, which is a retarded classical electron-electron propagator, satisfying a modified diffusion equation in the frequency domain [14,18] so that

$$\square\square(\square) = \square\frac{2e^2 D}{\square\hbar} C_{\square}(\mathbf{r},\mathbf{r}')\ \square\ \frac{\square G}{G_c}\ \mu\ \square\ln(1+\frac{\square_{\square}}{\square}) \quad (13)$$

4 CONCLUSION

We study the *influence of vacuum-fluctuation* in quasi-ballistic conduction in SWNT noting that this environmental condition also at low temperature introduce some dynamic disorder which involves, by means inelastic scattering [19], a *weak localization correction to the conductance*.

Appendix A LUTTINGER LIQUID: VERY BRIEF REVIEW

A Luttinger liquid (LL) is a one-dimensional (Fermi liquid) correlated electron state characterized by a parameter g that measures the strength of the interaction between electrons: strong repulsive interactions have $g << 1$, whereas $g = 1$ for the non-interacting electron gas (remembering that weakly interacting electrons in normal metal are described by quasiparticles of the Fermi liquid).

The LL's are very special in that they retain a Fermi surface enclosing the same k-space volume as that of free fermions, but there are no fermionic quasi-particles (like in normal Fermi liquids), their elementary excitations are bosonic collective charge and spin fluctuations dispersing with different velocities. An incoming electron decays into such charge and spin excitations which then spatially separate with time (*charge-spin separation*): the correlations between these excitations are anomalous and show up as interaction-dependent non-universal power laws in many physical properties where those of ordinary metals are characterized by universal (interaction-independent) powers. A list of such properties includes: 1) a continuous momentum distribution function $n(k)$, varying with as $|k \square k_F|^{\square}$ with an interaction-dependent exponent $\square$, and a pseudogap in the single-particle density of states $\mu\ |\square|^{\square}$, consequences of the non-existence of fermionic quasi-particles; 2) similar power-law behavior in all correlation functions (in those for charge or spin density wave fluctuations) with *universal scaling relations* between the different non-universal exponents, which depend only on one effective coupling constant per degree of freedom; 3) finite spin and charge response at small wave vectors and finite Drude weight in the conductivity; 4) spin-charge separation; persistent currents quantized in units of $2k_F$

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