Doping- and size-dependent suppression of tunneling in carbon nanotubes

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We study the effect of doping in the suppression of tunneling observed in multi-walled nanotubes, incorporating as well the influence of the finite dimensions of the system. A scaling approach allows us to encompass the different values of the critical exponent $\alpha$ measured for the tunneling density of states in carbon nanotubes. We predict that further reduction of $\alpha$ should be observed in multi-walled nanotubes with a sizeable amount of doping. In the case of nanotubes with a very large radius, we find a pronounced crossover between a high-energy regime with persistent quasiparticles and a low-energy regime with the properties of a one-dimensional conductor.

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During recent years there has been much interest in the investigation of the electronic properties of carbon nanotubes (CN) [1]. The reduced dimensionality of these systems leads to the appearance of unconventional effects, such as a suppression of the tunneling conductance at low energy scales. This has been interpreted as a signature of the so-called Luttinger liquid behavior [2,3], characterized by the absence of electron quasiparticles in the spectrum. Evidence of a power-law behavior in the tunneling density of states at low energies has been obtained from measurements in ropes [4], individual single-walled nanotubes (SWNT) [5] and multi-walled nanotubes (MWNT) [6].

In the Luttinger liquid picture, critical exponents of observables like the density of states are not universal and depend on the interaction strength. In the case of carbon nanotubes, this refers to the ubiquitous Coulomb interaction. However, a precise determination of the interaction strength is precluded by the fact that the electron-electron interaction is actually long-ranged, and it can be assimilated to a coupling constant, only after introducing a suitable infrared cutoff in the singular expression of the potential in momentum space. The Coulomb potential $1/|r|$ can be represented in three spatial dimensions as the Fourier transform of the propagator $1/k^2$. If the interaction is projected onto one spatial dimension, by integrating for instance the modes in the two transverse dimensions, then the Fourier transform has the usual logarithmic dependence on the momentum, $V_C(k) = (1/2\pi) \ln(k_c/k)$. In this approach, $k_c$ is the memory that the system keeps of the finite size of the transverse dimensions. We choose instead to integrate formally a number $3-D$ of dimensions, so that the long-range potential gets the representation

$$\frac{1}{|r|} = \int \frac{d^D k}{(2\pi)^D} e^{ikx} \frac{c(D)}{|k|^{D-1}} \quad (1)$$

where $c(D) = \Gamma((D-1)/2)/(2\sqrt{\pi})^{3-D}$. In the limit $D \to 1$, the expression of the potential in momentum space becomes

$$\frac{c(D)}{|k|^{D-1}} \approx \frac{1}{2\pi} \left( \frac{1}{D-1} - \ln(|k|) + \cdots \right) \quad (2)$$

This shows that $1/(D-1)$ corresponds actually to the logarithm of the high-energy cutoff $k_c$. In the RG framework, where all quantities are scaled down to low momenta, the dimensionless quantity $1/(D-1)$ has to be traded for the logarithm of the length of the system, measured in units of the nanotube finite radius.

The great advantage of dealing with the above representation is that the Coulomb interaction gives rise classically to a scale invariant theory at any dimension above $D = 1$, which allows to proceed with the RG program. It is only at $D = 1$ that the mentioned logarithmic dependence on the momentum leads to an imperfect scaling
behavior, making the use of the RG approach not quite appropriate. Then, we write the Hamiltonian for the linear branches of CN in the form

\[ H = v_F \sum_{\alpha \sigma} \int_0^\Lambda dp |p|^{D-1} \int d\Omega^\prime (2\pi)^D \Psi^\prime_{\alpha \sigma}(p) \sigma \cdot \Psi_{\alpha \sigma}(p) \]

\[ + e^2 \int_0^\Lambda dp |p|^{D-1} \int d\Omega^\prime (2\pi)^D \rho(p) \frac{c(D)}{|p|^{D-1}} \rho(-p) \]

(3)

where the \(\sigma_i\) matrices are defined formally by \(\{\sigma_i, \sigma_j\} = 2\delta_{ij}\) and \(\rho(p)\) are density operators made of the electron fields \(\Psi_{\alpha \sigma}(p)\), with \(\alpha\) labeling the Fermi point and \(\sigma\) the spin projection. The sum in Eq. (3) runs then over the usual four modes present in a single-walled nanotube, but it may include also the contribution from a large number of subbands in the case of a doped multi-walled nanotube.

We focus on the scaling properties of the model as the cutoff \(\Lambda\) is lowered, when a large number \(N\) of subbands contribute to the electronic properties down to the Fermi level. Each subband is labeled with a different quantum dimension around the nanotube. For this reason, the dominant processes are those where each scattered electron remains in the same linear branch. The main effect of the interaction is to dress the bare electron propagator with the polarization of the \(N\) different subbands given by

\[ \Pi(k, \omega_k) = 2Nb(D) \frac{v_F^2 - Dk^2}{|v_F^2 - k^2 - \omega_k^2|^{(3-D)/2}} \]

(4)

where \(b(D) = \frac{2}{(2\pi)^d} \frac{\Gamma((d+1)/2)}{\Gamma((d-1)/2)} \frac{\Gamma((d-3)/2)}{\Gamma((d+1)/2)} [13]\). The polarization (4) is the analytic continuation of the known result for two linear branches with opposite chirality, which we take away from \(D = 1\) in order to carry out a consistent regularization of the Coulomb interaction. After dressing the interaction with the polarization (4), the electron self-energy is given by the expression

\[ \Sigma(k, \omega_k) = -e^2 \int_0^\Lambda dp |p|^{D-1} \int d\Omega \frac{d\omega_p}{2\pi} G(k - p, \omega_k - \omega_p) \frac{1}{\epsilon_p - e^2 \Pi(p, \omega_p)} \]

(5)

The low-energy properties of the theory are investigated by taking the limit \(\Lambda \to 0\), where the self-energy \(\Sigma\) turns out to have terms linear in \(\omega_k\) and \(k\) that depend logarithmically on the cutoff. This is the signal that the scale of the electron wavefunction \(Z^{1/2}\) and the Fermi velocity \(v_F\) are renormalized at low energies. The divergent contributions to the electron propagator read

\[ \frac{1}{G} = \frac{1}{G_0} - \Sigma \approx Z^{-1} (\omega_k - v_F \sigma \cdot k) \]

\[ -Z^{-1} \frac{f(D)}{2N} \sum_{n=0}^{\infty} (-1)^n g^{n+1} \left( \frac{n(3-D)}{n(3-D) + 2} \omega_k \right) \]

\[ + \left( 1 - 2 \frac{n(3-D) + 1}{D n(3-D) + 2} \right) v_F \sigma \cdot k \] \(h_n(D)\log(\Lambda)\)

(6)

where \(g = 2Nb(D)c(D)v_F^2/v_F, h_n(D) = \frac{\Gamma(n(3-D)/2+1/2)}{\Gamma(n(3-D)/2+1)}\), and \(f(D) = -\pi^2 v_F^2 \frac{1}{D n(3-D) + 2}\).

The usual RG argument is that the renormalized propagator \(G\) must be a finite quantity, so that the divergent dependences on the cutoff \(\Lambda\) have to be reabsorbed in the scale of the wavefunction \(Z^{1/2}\) and the Fermi velocity \(v_F\) [14]. Under a differential variation of \(\Lambda\), \(Z^{1/2}\) is renormalized according to the equation

\[ \Lambda \frac{d}{d\Lambda} \log Z(\Lambda) = -\frac{f(D)}{2N} \sum_{n=0}^{\infty} (-1)^n g^{n+1} \frac{n(3-D)}{n(3-D) + 2} h_n(D) \]

(7)

The renormalization of \(v_F\) can be translated into that of the effective coupling \(g = 2Nb(D)c(D)v_F^2/v_F\), since the electron charge \(e\) is not renormalized in our model. The RG equation for \(g\) becomes

\[ \Lambda \frac{d}{d\Lambda} g(\Lambda) \approx \frac{1}{2N} (D-1) g \left( 1 - \frac{1}{\sqrt{1+g}} \right) \]

(8)

We are now in a position to study the influence of the long-range Coulomb interaction in the limit \(D \to 1\). For this purpose, we start by considering the RG equation (8). The series showing in the r.h.s. can be summed up at \(D = 1\), the flow equation taking then the following form in the neighborhood of that point:

\[ \Lambda \frac{d}{d\Lambda} g(\Lambda) \approx \frac{1}{2N} (D-1) g \left( 1 - \frac{1}{\sqrt{1+g}} \right) \]

(9)

It follows from Eq. (9) that, at \(D = 1\), there is formally a line of fixed-points covering all values of the interaction strength. However, we still have to take into account that the effective coupling \(g(D)\) becomes singular in the limit \(D \to 1\). We can shuffle this divergence into the initial value of the coupling, \(g_0(D)\), which turns out to have near \(D = 1\) the asymptotic behavior

\[ g_0(D) \approx N \frac{e^2}{\pi v_F} \frac{1}{D-1} \]

(10)

Then, by matching the behavior of \(g_0(D)\) with that of Eq. (9), we observe that the \(D - 1\) factor in the r.h.s. of the RG equation is not completely canceled out in the limit \(D \to 1\). This shows in a rigorous way that the bare 1D long-range interaction is a RG fixed-point for arbitrary values of the interaction strength.

We consider next the RG equation (7) for the electron wavefunction scale in the limit \(D \to 1\). The series in the r.h.s. can be also summed up at \(D = 1\), with the result that the scaling equation in that limit reads

\[ \Lambda \frac{d}{d\Lambda} \log Z(\Lambda) \approx \frac{1}{4N} \left( \sqrt{1+g} + \frac{1}{\sqrt{1+g} - 2} \right) \]

(11)
The function in the r.h.s. of Eq. (11) coincides with the anomalous electron dimension found in the exact solution of the Luttinger model [15,16]. This ensures that the RG approach is a sensible way to obtain the low-energy properties of the model. We have to bear in mind that our description introduces however two important differences with respect to the usual treatment of 1D interacting electrons. On the one hand, the slight deviation of the model from \( D = 1 \) allows to control the approach to the bare long-range interaction as the length of the system is increased. On the other hand, we have also incorporated the effect of the number \( N \) of subbands that contribute at low energies, in order to account for the influence of doping in MWNT.

With the RG approach we can face two different experimental conditions, depending on the magnitude of the typical energy scale involved in the measurement process, as compared to the spacing between subbands in the nanotube sample. When the latter is larger than the temperature or bias voltage applied to the sample, we are in a situation where the number of subbands \( N \) can be taken as constant along the RG flow. Otherwise, for large enough temperature or bias voltage, the number of subbands that contribute at the scale of the high-energy cutoff is a decreasing variable as \( \Lambda \to 0 \). We deal separately with the two instances in what follows.

**RG approach with a constant number \( N \) of subbands.**—
In transport experiments, the typical scale of temperature or bias voltage lies usually below the scale of the spacing between subbands. This has been so, even in the measurements made in MWNT, where the spacing corresponding to a typical diameter \( d \approx 17 \text{ nm} \) is as small as \( h v_F/d \approx 29 \text{ meV} \). In these conditions, the only subbands that contribute to the properties measured experimentally are those crossing the Fermi level.

We apply then Eqs. (10) and (11) to confront the experimental results on the tunneling density of states gathered from different nanotube samples. Starting with the measurements made in SWNT, we take a number of subbands \( N = 2 \) in the equations and adjust the deviation from \( D = 1 \) in accordance to the length of the experimental sample. Following the argument below Eq. (2), we use the correspondence \( 1/(D - 1) \approx \ln(L/d) \), \( L \) being the nanotube length and \( d \) the nanotube diameter. A suitable choice corresponding to the experiments reported in Ref. [5] is \( L/d \approx 10^3 \), which gives in turn \( D \approx 1.14 \).

The measurements of the tunneling density of states in SWNT have shown a power-law dependence on energy, with values of the critical exponent \( \alpha \) accumulating around \( \approx 0.35 \) [4,5]. We have represented in Fig. 1 the estimates obtained from the r.h.s. of Eq. (11), for small values of \( D - 1 \). The values of \( \alpha \) have a smooth dependence on the length \( L \) of the system and fall around \( \alpha \approx 0.35 \) for \( N = 2 \) and \( D \approx 1.14 \), with a reasonable choice of the coupling \( e^2/\pi^2 v_F \approx 1.5 \).

Our results show also an overall agreement with the exponents measured in MWNT. It has been noticed that such systems are significantly doped, so that a large number of subbands are found at the Fermi level. The experimental conditions refer to a situation where \( N \approx 5 - 10 \) (without taking into account the spin degeneracy). It has been reported that the values of the critical exponent \( \alpha \) measured in 11 different samples range from 0.24 to 0.37 [6]. This variation can be accounted for within our RG approach by assuming that the number of subbands used in the renormalization may shift from \( N = 2 \) to \( N = 10 \). Part of the drift observed in the critical exponent may be also due to the smaller aspect ratio of MWNT, although this fact is difficult to assess given the lack of information about the total length of the experimental samples.

![FIG. 1. Estimates of the exponent \( \alpha \) from the r.h.s. of Eq. (11), for \( e^2/\pi^2 v_F \approx 1.5 \). The different curves correspond, from top to bottom, to \( D = 1.14, 1.16 \) and 1.18.](image)

We show then that the suppression of tunneling in MWNT can be softened by increasing the doping level. Our results may be also relevant in general for nanotubes of large radius where there are a large number of subbands crossing the Fermi level. These instances can be considered as midway in the process of making contact with the physical properties of a graphene sheet. This requires taking systems with larger transverse size, what in turn may lead to a situation where the spacing between subbands is smaller than the typical energy scale in the experimental measurements. One has then to change slightly the computational scheme, as discussed below.

**RG approach with a cutoff-dependent number of subbands \( N(\Lambda) \).**—In samples of a very large diameter, one may envisage conditions where the temperature or the bias voltage are much larger than the subband spacing in the nanotube. The RG approach can be still implemented, but taking into account that the number of subbands contributing in the partial integration of modes at energy \( \Lambda \) depends on the value of the high-energy cutoff. Let us suppose for simplicity that the system is at half-filling, with the typical structure of two subbands
crossing at the Fermi level. For not too large energies, the number of subbands crossing the energy level $\varepsilon$ has then a linear dependence on $\varepsilon$, $N(\varepsilon) = N_0 + n_p \varepsilon$, where $N_0 = 2$ is the number of subbands at the Fermi level.

We obtain the scaling of the quasiparticle weight $Z$ and the different observables by imposing a dependence of $N$ on the cutoff $\Lambda$ according to the above formula. This description yields a sensible prediction for experiments where the average effect of a large number of subbands is measured. The dependence of the quasiparticle weight $Z$ on energy as the cutoff is sent towards the Fermi level is represented in Fig. 2, for different values of $n_p$. In the present instance, the dominant contribution to the power-law behavior of the tunneling density of states comes from the number of subbands varying with the energy scale. This sets the value of $\alpha$ close to 1 from the start, what is the natural way of recovering the characteristic linear density of states of a graphite layer from our 1D point of view.

![Graph showing energy dependence of quasiparticle weight](image)

**FIG. 2.** Energy dependence of the quasiparticle weight $Z$ at dimensions 6/5 and 8/7, for different values of $n_p$.

We observe from the results in Fig. 2 that the quasiparticle weight $Z$ tends to have a flat behavior at high energies for large values of the density of subbands $n_p$. This is in contrast to the rapid decrease signaling the typical power-law behavior for small values of $n_p$. In the curves for $n_p = 100$ and $n_p = 1000$, we see the existence of a crossover between a regime with persistent quasiparticles and another characteristic of the Luttinger liquid behavior. The physical interpretation is that, for high energies above the crossover scale, the system has similar properties to the 2D graphene, while one has to look at sufficiently small energy scales (or large length scales) to measure the properties of the 1D wire.

We have obtained several results that may be checked against future measurements carried out in MWNT and nanotubes of very large radius. We predict that the ex-

ponent giving the power-law behavior of the tunneling density of states may suffer a significant reduction upon doping those systems, with the possibility of reaching values as small as 0.1 for $N \approx 40$. We have also shown that, when dealing with nanotubes of very large radius, there is a high-energy regime with persistent electron quasiparticles which has properties closer to 2D graphene than to the Luttinger liquid. We believe such features may be of interest when developing carbon-based devices made of graphene and nanotube structures with different shapes.

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