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The role of the geometry in multiwall carbon nanotube interconnects

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We develop an approach to calculate the electron spectrum of metallic multiwall carbon nanotubes (MWNT) with an arbitrary number of coaxial layers. The approach is based on the model with singular attractive potential of equidistant conductive cylinders and includes the presence of a geometrical potential. The knowledge of the one-electron spectrum allows us to calculate the number of electrically active channels, N_{ch} , in MWNT in the ideal case where all the shells are contacted to the electrodes. Starting from the dependence of N_{ch} on the temperature and on the radii of both the innermost and outermost tube we will be able to discuss the potential performances of MWNT interconnects. With the aim of designing carbon based nanointerconnects, we demonstrate that, for small innermost radius MWNT, the presence of the geometrical potential can be quite relevant, when all the shells are contacted to the electrodes, while the intershell tunneling can be quite relevant in determining N_{ch} , when the radius of the outermost shell becomes of the order of hundreds of nanometers. © 2010 American Institute of Physics. [doi:10.1063/1.3491028]

I. INTRODUCTION

Carbon nanotubes (CNT) are prototype one-dimensional (1D) carbon systems and represent promising candidates for future applications, such as new conductors for nanoelectronics,¹ cold electron sources for field emission,² and new materials for nanomechanics, because they are extremely stiff and resistant to bending.³

They are basically rolled up sheets of graphene forming tubes [see Fig. 1] that are only nanometers in diameter and have length up to some microns. CNT may be grown as single-walled (SWNT) or multiwalled ones (MWNT, typically made of several concentrically arranged graphene sheets). They exhibit semiconducting or metallic properties, depending on the helicity of the carbon rings around the tubule.⁴

Since the current carrying capacity of CNTs did not degrade after 350 h at current densities of 10^{10} A/cm² at 250 °C (Ref. 5) and their thermal conductivity^{6,7} is about 1700–3000 W/mK, in recent years CNTs were proposed to develop an innovative cost-effective and reliable technological solution for high-performance next generation nanointerconnects beyond the limit of current technology.⁸ CNTs interconnects will have high-transmission speed, high current density, exceptional mechanical and thermal properties, optimum signal, and power integrity.⁸

Interconnects are considered one of the grandest challenges that gigascale integration faces, because of the delay they add to critical paths, the power they dissipate, the noise and jitter they induce on one another, and their vulnerability to electromigration. CNT show great potential in addressing some of the major interconnect challenges in future generations of technology, when copper conductivity will degrade substantially because of size effects.⁹ In fact, the copper interconnect is actually used with minimum feature sizes down

to 130 nm.^{10,11} However, many problems are due to the electrical resistivity of copper, which increases with a decrease in dimensions, due to electron surface scattering and grain-boundary scattering,^{12,13} and to the electromigration failure of copper lines.^{14–16} Such size effects arise from interface roughness and small grain size, which are hard to overcome.¹³ Thus, in the last decade CNT have been envisioned as a possible replacement for copper electrical interconnects for future gigascale integration.^{5,17–21} Especially, highly aligned parallel nanotube architectures comprising all-metallic SWNT are expected to outperform copper, in terms of failure current density, power dissipation, and on-chip signal transfer delays.^{22–26}

The electronic properties of a CNT as an interconnect strongly depend on the number of electrically active channels, N_{ch} . This number, which is determined by the nature of the metallic contacts, is the fundamental physical parameter needed, in order to evaluate the main transport properties of a MWNT.^{8,25}

In this paper we calculate N_{ch} in MWNT in the ideal case when all shells are contacted to the electrodes by focusing on the effects of both the geometrical potential and the intertube coupling.

The remainder of the paper is organized as follows. In Sec. II, we introduce the models usually adopted to evaluate the electron spectrum and effective number of channels of CNT in the ballistic limit. In Sec. III, we report the results obtained by including the so called radial corrections. Some details about the usual approach used to evaluate N_{ch} applying the Landauer formula are reported in Appendix A, while in Appendix B we present some technicalities about the calculations of the spectra.

II. NUMBER OF CHANNELS AND INTRINSIC RESISTANCE

Even under the hypothesis of ballistic conduction, that is if the length of CNT is lower than the mean free path, l_{mfp} , a

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FIG. 1. (Color online) SWNTs are basically rolled up sheets of graphite forming tubes that are only nanometers in diameter and have length up to some microns, while MWNTs are typically made of several concentrically arranged graphene sheets. The intershell distance δ is constant and equal to the intergraphene distance of 0.34 nm, while the number of shells can be evaluated, starting from the innermost tube radius, R_i and the outermost tube one R_o , as $(R_o - R_i) / \delta$. MWNT may have diameters in a wide range from a few to hundreds of nanometers. SWNT can be thought of, as the fundamental cylindrical structure, forming the building blocks of both MWNTs and the arrays of SWNTs, also in bundles.

single metallic shell (or a metallic SWNT) presents an intrinsic resistance $\bar{R}_i$ on the order of $k\Omega$, accounting for the effect of the voltage drop at the CNT-metallic electrode interfaces,

$$\bar{R}_i = \frac{h}{2N_{ch}e^2}, \quad (1)$$

where N_{ch} is the number of electrically active channels. Equation (1) represents the lowest theoretical and measurable equivalent dc resistance of a metallic SWNT.

Obviously a crucial role in determining the value of N_{ch} is played by the nature of the metallic contacts. Although initially most experiments indicated that only the outer shell in a MWNT conducts, in recent years it has been shown that all shells can conduct, provided they are properly connected to the contacts.^{27–29} Moreover, in general, contacts do not behave in an ideal way and, in the case of imperfect contacts, an additional resistance should be added to $\bar{R}_i$. In order to achieve low resistances, not only should all shells conduct, but the contact resistance for each shell should also be relatively small. In this case MWNT may be adopted for large-scale integration. Next, we consider MWNT in the ideal case where all the shells are contacted to the electrodes.

In some previous calculations^{8,25} of N_{ch} at least two factors were neglected.

- (I) When the Schrödinger equation for a spinless charged particle constrained to a curved surface is derived using a thin-layer procedure, the latter gives rise to the well-known geometric potential.^{30–32} This extra energy can be usually disregarded in SWNT, whereas it can give relevant effects on MWNT, when all the shells are contacted.
- (II) In general, the one-electron spectrum in MWNT depends on the presence of the neighboring shells. In fact, the intertube coupling in MWNT was demonstrated to be essential, for the interpretation of experimental data on electric transport properties of MWNT.^{33,34}

In the remainder of the section, we develop a theoretical approach useful to calculate the electron spectrum of metallic MWNT, with an arbitrary number of coaxial layers. This

approach assumes the metallic MWNT as a set of equidistant coaxial cylinders with attractive Kronig–Penney-type potential along the radius and studies the electron states of such a system. In this way the electron tunneling between the adjacent tubes is taken into account and the hopping of electrons between the tubes leads to splitting of degenerate energy levels. In this model the chirality of each internal shell is neglected, while the Dirac-like behavior, typical of electrons in carbon materials is taken into account. In this sense the model used here improves the one proposed in Ref. 32, where the electrons have a parabolic dispersion. The effects of the chirality can be obviously less relevant, when large radius MWNT with several shells are taken into account.

A. Bandstructure of CNT and Dirac fermions

The unique electronic properties of CNT are due to their diameter and chiral angle (helicity), parameterized by a roll-up (wrapping) vector $\vec{w} = (n_w, m_w)$. This vector corresponds to the periodic boundary conditions and gives us the dispersion relations of the 1D bands.

Usually the electronic spectra of graphite nanotubes were calculated in the tight-binding approximation, which starts from the microscopic structure of the hexagonal graphite lattice and takes into account only interactions with the nearest neighbors.

An alternative technique,³⁵ known as $\mathbf{k} \cdot \mathbf{p}$, is useful to obtain electronic spectra of carbon based materials. This approach is based on the equation which describes the electronic states near a K point, $\pm K_s = \pm (4\pi) / (3\sqrt{a_0})$ of two-dimensional graphite, where a_0 is the C–C distance. Thus, the 1D bandstructure, for momenta near $\pm K_s$, is³⁶

$$\varepsilon_0(m, \vec{w}, k) \approx \pm \frac{v_F \hbar}{R} \sqrt{\left(\frac{m_w - n_w + 3m}{3} \right)^2 + R^2 (k \pm K_s)^2}, \quad (2)$$

where R is the tube radius and v_F represents the Fermi velocity, given by $v_F = 3ta/2$, with a value $v_F \approx 1 \times 10^6$ m/s.³⁷

Thus, we obtain that just 1/3 of the possible nanotubes are metallic, when the condition $m_w - n_w = 3q$, with q integer, is fulfilled. For a metallic CNT (e.g., the armchair one with $m_w = n_w$), we obtain that the energy vanishes, for two differ-

ent values of the longitudinal momentum $\varepsilon_0(\pm K_s)=0$. In conclusion, each SWNT can be conducting or not, depending on its chirality. However, the larger is the SWNT diameter, the higher results the probability that a tube be conducting, because the number of conducting channels of a quasimetallic carbon shell increases with the diameter of the tube.

The dispersion law $\varepsilon_0(m, k)$, in the case of undoped metallic nanotubes, is linear near the crossing values $\pm K_s$. The linear dispersion relation holds for energy scales $E < D$, with the bandwidth cutoff scale $D \sim v_F \hbar / R \approx 70/R$ meV nm.

Starting from Eq. (2), we can develop a Dirac-like theory for CNT (Ref. 38) and the Hamiltonian, near a Fermi point, reads

$$H_D = v_F(\hat{\sigma}_y \pi_\varphi + \hat{\sigma}_x \pi_y), \quad (3)$$

where $\hat{\sigma}_i$ are the Pauli matrices, $\pi_\varphi = \frac{L_y}{R} = -i \frac{\hbar}{R} \frac{\partial}{\partial \varphi}$ corresponds to the momentum along the circumference of the nanotube while $\pi_y = p_y \pm \hbar K_s$ is the momentum along the axis. For metallic CNTs, such as the armchair ones, the problem in Eq. (3) has periodic boundary conditions and a factor $e^{im\varphi}$ appears in the wave function. For semiconducting CNTs ($m_w \neq n_w$) we have to define *quasiperiodic boundary conditions*,³⁹ corresponding to a phase factor in the wave function $e^{i(m+m_w-n_w/3)\varphi}$.

Thus, we can trivially obtain the spinorial eigenfunctions, while the eigenenergies are given by Eq. (2).

B. Number of channels for a SWNT

Following the seminal paper of Naeemi and Meindl,²⁵ we can evaluate the number of conducting channels for a SWNT (or for each shell of a MWNT).

The number of channels $N_{ch}(R)$ for a shell with radius R at $T=300$ K, assuming that shells have random chiralities (i.e., statistically 1/3 of the shells are metallic and the rest semiconducting^{1,40}), can be approximated by⁴¹

$$\begin{aligned} N_{ch}(R) &= aR + b; \quad R > 1.5 \text{ nm} \Leftrightarrow N_{ch}(R) \sim 2\bar{a}R_T \\ &+ \bar{b} \quad R > R_T/T, \\ N_{ch}(R) &\sim 2/3; \quad R < 1.5 \text{ nm} \Leftrightarrow N_{ch}(R) \sim 2/3 \\ &R < R_T/T, \end{aligned} \quad (4)$$

where $\bar{a}$ is $3.87 \times 10^{-4} \text{ nm}^{-1} \text{ K}^{-1}$, $\bar{b}$ is 0.2, and $R_T = 650 \text{ nm K}$.

Details about the calculations to obtain Eq. (4) are reported in Appendix A. At zero temperature ($T=0$ K), all energy states below the Fermi level are occupied, and the ones above it are free. Completely full or empty subbands cannot contribute to conduction; hence, only those that cross the Fermi level determine the number of channels. At temperatures above 0 K, electrons are distributed according to the Fermi function, and all subbands contribute to conduction according to the Fermi function.

A key role in the calculations is played by the number of conducting channels for each shell, at a given energy $N_{eff}(\varepsilon)$. This number has to be written following the single-electron spectrum, e.g., Equation (2), as

$$N_{eff}(\varepsilon) = \text{Int} \left(\frac{R\varepsilon}{v_F \hbar} - \alpha_w + 1 \right) \sim \frac{R\varepsilon}{v_F \hbar}, \quad (5)$$

where $\alpha_w = (m_w - n_w)/3$ can be 0, 1/3, or 2/3 according to the chirality. We report the derivation of Eq. (4) from Eq. (5) [see Eq. (A6)] in Appendix A. There, the Landauer approach is discussed as well, also in the case of more subbands contributing to conduction.⁴² For interconnect applications, we are more interested in the low-bias conductance, because the electric field along interconnects is typically small.⁴³ Equation (4) is, therefore, accurate enough, for nanotube interconnects.

C. Multiwall tube

In Fig. 1 the schematic plot of a MWNT is reported: the intershell distance δ is constant and equal to the intergraphene distance of 0.34 nm, whereas the number of shells, N_{sh} , can be related to the inner, R_i , and outer, R_o , radius of the MWNT as $N_{sh} = (R_o - R_i)/\delta$.

The independent shell approximation is based on the hypothesis that the intershell hopping in a MWNT is totally negligible. Thus, the Eq. (4), derived for isolated shells, can be applied. Starting from the latter equation, the number of channels for a MWNT, with external radius R_o and inner radius R_i was calculated²⁵ assuming $R_i > 1.5 \text{ nm}$

$$\begin{aligned} N_{chan} &= \left(1 + \frac{R_o - R_i}{\delta} \right) \left[\frac{a}{2} (R_o + R_i) + b \right] \sim a \frac{R_o^2 - R_i^2}{2\delta} \\ &+ b \frac{R_o - R_i}{\delta}. \end{aligned} \quad (6)$$

The right hand side of the equation can be easily obtained by integrating Eq. (4), i.e., by using the continuum approximation. The known formula on the left hand side comes from the sum over shells and includes an extra term, usually negligible for large radius MWNT. For more details see Appendix B and Eqs. (B1) and (B2).

D. Corrections to the model: the radial terms

In the discussions reported above, the effects of the radial part of the Hamiltonian are totally neglected. The inclusion of this part in the Hamiltonian yields some additive terms, that could be relevant in the exact evaluation of the number of conducting channels, both for a single and a multiwall CNT.

1. The geometrical term

The Schrödinger equation, for a spinless charged particle constrained to a curved surface, was derived in a recent letter³¹ by Ferrari and Cuoghi. However, the presence of a geometrical term which depends only on the radius of the tube,

$$H_g \equiv - \frac{\hbar^2}{8mR^2},$$

was already discussed in the past.³²

2. The intertube coupling

The authors of Ref. 32 developed a general approach to calculations of the electron spectrum of metallic MWNT, with an arbitrary number of coaxial layers. It is based on the model where coaxial graphite shells were treated as continuous conducting cylinders with singular attractive potential,

$$U(r) = \sum_{n=0}^{N_{shell}-1} U_0(r - R_m - n\delta).$$

Here N_{shell} is the number of cylinders and R_m is the radius of the m th shell. Thus electrons are held to each cylinder by a singular attractive potential, given by a potential well of width $W \sim 0.02$ nm and $U_0(0) = -\hbar^2/(mW^2)$, corresponding to a binding energy $E_b = U_0(0)/2$. The single-electron Hamiltonian takes the form

$$H = \frac{p_r^2}{2m} + U(r) + \frac{p_\phi^2}{2mr^2} + \frac{p_y^2}{2m}. \quad (7)$$

The main problem in using this approximation, for the calculation of the integrated circuits (IC) properties of MWNT, is due to the inverse quadratic dependence on the radius of the intersubband gap. The latter behavior disagrees with the one predicted and observed for CNT.

A better approximation can be obtained by developing the approach based on the Dirac fermions, thus Eq. (7) becomes

$$H = \left[\frac{p_r^2}{2m} + U(r) \right] \hat{1} + v_F [\hat{\sigma}_y \pi_\phi + \hat{\sigma}_x \pi_y], \quad (8)$$

where $\hat{1}$ is the 2×2 identity matrix.

III. RESULTS

A. The geometrical correction to the single tube

From Eq. (7) we obtain the electronic energy spectrum for an isolated SWNT as

$$\varepsilon_{k_y, m, R} = -E_b - \frac{\hbar^2}{8m^* R^2} + \frac{p_y^2}{2m^*} + \frac{\hbar^2 m^2}{2m^* R^2}, \quad (9)$$

where the first negative term is the binding energy of the electron in the potential well which does not depend on the form of the graphite layer. The last two terms yield the kinetic energy of the electron: the longitudinal part $\propto p_y$ varies continuously, whereas the angular component $\propto m^2$ is quantized.

Following Ref. 32 the scale of quantization energies reads

$$E_m \sim \frac{40}{R^2} \text{ meV nm}^2; \quad E_g \sim \frac{10}{R^2} \text{ meV nm}^2,$$

for the angular kinetic and the geometrical term, respectively. Since the latter term depends only on the radius of the tube, it follows that electrons are bound to the tube more strongly than to the plane.

The results obtained in Ref. 32 can be extended to the Dirac fermions model. From Eq. (8) we can obtain the electronic energy spectrum for an isolated SWNT, within the

Dirac fermion approximation. We use the so called strong coupling approximation usually adopted in the semiclassical solutions of the spin Hamiltonians.⁴⁴ We introduce the eigenfunctions in the form $u_{m, k_y, n^*}(r) \hat{\Psi}_{m, k}(\phi, y)$, and we obtain

$$\varepsilon_{k_y, m, R} \sim -E_b - \frac{\hbar^2}{2m^* R^2} \pm v_F \sqrt{\frac{\hbar^2(m - \alpha_w)^2}{R^2} + p_y^2}. \quad (10)$$

Following the case discussed above, the scale of quantization energies is

$$E_m \sim \frac{70}{R} \text{ meV nm}; \quad E_g = \frac{\lambda}{R^2} \sim \frac{10}{R^2} \text{ meV nm}^2,$$

for the angular kinetic and for the geometrical term, respectively.

The bottom subbands energies are now shifted by the presence of the geometrical term, according to the plot reported in the top panels of Fig. 2. In Fig. 2 top left the effects due to the geometrical term are reported in the van Hove singularities (bottom of the subbands), for different radius CNT, according to Eq. (8). The geometrical term shifts the bandstructure significantly for small radius CNT, while the contribution becomes negligible for large radius CNT. A schematic representation of the bandstructure for a seven shell MWNT is reported in the top right panel, where the effects of the geometrical term are emphasized for each shell.

However, for a SWNT (or for a shell of a MWNT) with radius $R > 2$ nm, the effects are quite small, especially at temperatures of the order of the room one. In fact, since $k_B = 8.6 \times 10^{-2}$ meV/K, for $T \sim 300$ K the thermal energy $k_B T$ can be assumed as 25 meV, while E_g results below 2.5 for $R > 2$ nm and can be neglected.

However, an intrinsic doping due to the geometrical energy shift can be relevant, when the innermost tube radius becomes of the order of a few nanometers. In fact, when all the shells of a MWNT are connected to a metallic contact, the Fermi level is shifted and is the same for all the internal CNT. This is equivalent to a doping effect on the CNT.

Thus, we are able to analyze the effects of the radial term, in determining the number of open channels in a MWNT.

In the bottom panels of Fig. 2 the calculated numbers of conducting channels as a function of temperature are reported, according to Eqs. (A4) and (A5), for MWNT with 20 shells and different inner radius. The Fermi energy (i.e., the chemical potential of the contacts) is supposed to be fixed to the Fermi level of the innermost tube. It follows that the N_{ch} versus T behavior deviates from the ideal linear case, when the innermost tube is thin, while the continuum approximation plays well, when the innermost radius is above a few nanometers.

The corrections due to the geometrical term, relevant just for a small innermost tube radius, give also a reduction in the value of the parameter a in Eq. (4).

FIG. 2. (Color online) (Top left) The van Hove singularities (bottom of the subbands) for different radius CNT. The geometrical term shifts the bandstructure significantly for small radius CNT, while the contribution becomes negligible for large radius CNT. (Top right) Schematic representation of the bandstructure for a 7 shell MWNT. We report both the shell circumferences and the corresponding bandstructure. (Bottom) The calculated number of conducting channels for MWNT with 20 shells and different inner radius vs temperature. The Fermi energy (the chemical potential of the contacts) is supposed to be fixed to the Fermi level of the innermost tube. It follows that the N_{ch} vs T behavior deviates from the ideal linear case, when the innermost tube is thin (left panel with $R_i = 0.5$ nm), while the continuum approximation [see Eq. (4)] plays well, when the innermost radius is above a few nanometers (right panel with $R_i = 5$ nm).

B. Interwall tunneling

In this section we suppose that the electrons are trapped in the graphene layers corresponding to the CNT by a strong confining potential.

For the s th shell, with radius R_s , the single particle wave function can be approximated as

$$\psi_{k,m}^s \sim N e^{iky + i(m - \alpha_w)\varphi} u(r - R_s),$$

where $u(r - R_s)$ is a function strongly localized near R_s , while the centrifugal corrections to the radial part, δR , are small, as $(W/R)^4 R$ can be neglected.

The whole multilayer Hamiltonian can now be written as

$$H_{ML} = \int dk_y \sum_m \left(\sum_{s=1}^{N_{shell}} \sum_{\sigma=1}^{N_{shell}} \varepsilon_{k_y, m}^s |\psi_{k, m}^s\rangle \langle \psi_{k, m}^\sigma| \delta_{s, \sigma} + U_{s, \sigma} |\psi_{k, m}^s\rangle \langle \psi_{k, m}^\sigma| \right), \quad (11)$$

where, according Ref. 32, $U_{s, \sigma}$ can be evaluated as

$$U_{s, \sigma} \sim \frac{\hbar^2}{2m^* W^2} e^{-(|R_s - R_\sigma|/W)} = u_0 e^{-(|s - \sigma| \delta W)}.$$

More details about the calculations are reported in Appendix B. The results can be summarized in a formula for the bottom subbands energies of a MWNT. For a metallic shell and for $|m| > 0$ we obtain

TABLE I. Values of the numerically calculated α (meV), β (meV/nm), and γ (meV/nm²) parameters for different values of the inner and outer radius in nanometers.

R_i	R_o	N_{sh}	α	β	γ	$\Delta\varepsilon/\varepsilon$
10	11.7	5	0.001 3	−0.000 35	0.000 021	0.000 015 997 9
10	27.0	50	0.000 37	−0.000 051	1.6×10^{-6}	0.000 199 94
10	180.0	500	0.000 41	−0.000 015	9.5×10^{-8}	0.059 883 8
55	56.7	5	0.29	−0.012	0.00013	0.001 864 02
55	72.0	50	0.009 3	−0.000 33	2.9×10^{-6}	0.003 821 68
55	225.0	500	0.001 9	−0.000 036	1.4×10^{-7}	0.117 005
100	101.7	5	1.7	−0.040	0.000 23	0.010 785
100	117.0	50	0.047	−0.000 97	5.0×10^{-6}	0.016 428 8
100	270.0	500	0.005 1	−0.000 066	2.0×10^{-7}	0.202 235
145	146.7	5	−46.0	0.62	−0.002 1	0.032 403 7
145	162.0	50	0.13	−0.001 9	7.1×10^{-6}	0.043 646 1
145	315.0	500	0.011	−0.000 11	2.6×10^{-7}	0.321 2
190	191.7	5	-1.4×10^2	1.4	−0.003 6	0.072 344 9
190	207.0	50	0.29	−0.003 3	9.2×10^{-6}	0.091 098 2
190	360.0	500	0.020	−0.000 17	3.3×10^{-7}	0.479 523

$$\varepsilon_{m,R_s,R_i,R_o} \sim \frac{\hbar v_F}{R_s} |m| - \frac{\lambda}{R_s^2} - \frac{1}{|m|} (\alpha + \beta R_s + \gamma R_s^2), \quad (12)$$

with α , β , and γ depending on R_o and R_i . The values of the parameters in Eq. (12) are reported in the Table I, where we also report the value of $\Delta\varepsilon/\varepsilon$ for the outermost shell.

The number of conducting channels for each shell can be written by correcting Eq. (5). Thus, following the approach reported in Appendix A, we are able to evaluate the number of electrically active channels, N_{ch} .

In Fig. 3 we report the number of conduction channels, for different geometries of MWNT calculated at $T=300$ K. These CNT differ both for the inner radii (from 10 to 200 nm) and for the number of shells (from 5 to 50). The results reported show that the effects of the intershell hopping cannot be disregarded, when the radius (and/or the number of shell) becomes too large. The main effect of the increased

number of shells and the quadratic corrections to the dependence of N_{ch} on R are clearly shown in the right and left panels of Fig. 3 respectively.

IV. CONCLUSIONS

The performance and power dissipation of IC are largely affected by interconnects. CNTs show a great potential in addressing some of the major interconnect challenges in future generations of technology, when copper conductivity will degrade substantially because of size effects.

With the aim of determining the electronic properties of a MWNT as an interconnect, we have discussed a detailed calculation of the number of electrically active channels, N_{ch} for MWNTs in the ideal case where all the shells are contacted to the electrodes by including the effects of the radial terms of the Hamiltonian, usually disregarded.

At first, we have shown that an intrinsic doping due to the geometrical energy shift can be relevant, when the inner-

FIG. 3. (Color online) Number of conduction channels for different geometries of MWNT, calculated at $T=300$ K. CNT differ both for the inner radii (from 10 to 200 nm) and for the number of shells (from 5 to 50). The dashed line are obtained from Eq. (6), $N_{ch} \propto AR_i N_s + BN_s^2$, neglecting the intershell coupling. On the left, a quadratic deviation from this behavior is clearly shown.

most tube radius becomes of the order of a few nanometers. In fact, when all shells of a MWNT are connected to a metallic contact, the Fermi level is shifted and is the same for all the internal CNT. This is equivalent to a doping effect on the CNT.

Then, we have developed an approach to calculate the electron spectrum of metallic MWNT with an arbitrary number of coaxial layers by including the intertube coupling. We have demonstrated that the intershell tunneling can be quite relevant in determining N_{ch} , when the radius of the outermost shell becomes of the order of hundreds of nanometers. The model, where the MWNT is treated as a lattice along the radius, improves the one derived for isolated shells, with band structures unaffected by each other, and it could also be extended to the CNT ropes and bundles, by emphasizing the effects of intertube hopping.

Starting from our calculation, compact physical models can be developed to determine the ultimate potential performances of MWNT, with various diameters and lengths, and compare them with copper wires and SWNT bundles. These results offer important guidelines on which kind of nanotubes needs to be developed, for various interconnect applications. The calculations developed in the limit of ballistic conduction, has to be taken as the starting point of a more detailed discussion, which includes the effects of the disorder, when the length of the Interconnect becomes much longer than the mean free path.

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APPENDIX A: CONDUCTANCE CALCULATIONS

1. BALLISTIC TRANSPORT AND LANDAUER FORMULA

In order to study the transport properties of a 1D nanodevice subject to a constant, low-bias voltage (linear regime), we calculate the zero temperature conductance G based on the Landauer formula. The latter formula works in the ballistic transport regime, where scattering with impurities can be neglected and the dimensions of the sample are reduced below the mean free path of the electrons. We have

$$G = \frac{e^2}{h} \sum_{n', n=0}^M \sum_{\sigma', \sigma} T_{n'n}^{\sigma'\sigma}, \quad (\text{A1})$$

where $T_{n'n}^{\sigma'\sigma}$ denotes the quantum probability of transmission between incoming (n, σ) and outgoing (n', σ') asymptotic states defined on semi-infinite ballistic leads. The labels n, n' and σ, σ' refer to the corresponding mode and spin quantum numbers, respectively. Here the spin independent case is presented, where the sum over the spins gives a degeneracy factor 2.

The Landauer formula in the form of Eq. (A1) works just at $T=0$, while a more general formulation at finite tem-

peratures has to take into account the width of the distribution of injected electrons. Thus, the conductance at finite T is given by⁴⁵

$$G = -(e^2/h) \sum_{\gamma} \int_0^{\infty} d\varepsilon \frac{\partial f(\varepsilon, \varepsilon_F, T)}{\partial \varepsilon} |T_{\gamma}(\varepsilon)|^2, \quad (\text{A2})$$

where f denotes the Fermi distribution function, T is the temperature and

$$w(\varepsilon, \varepsilon_F, T) = - \frac{\partial f(\varepsilon, \varepsilon_F, T)}{\partial \varepsilon},$$

is often referred to, as the broadening function. Here, γ represents all quantum numbers (m, s , etc.).

In the limit of perfect transport, the transmissions can be written as

$$|T_{\gamma}(\varepsilon)|^2 = \Theta_H(\varepsilon - \varepsilon_{\gamma}), \quad (\text{A3})$$

where $\varepsilon \Theta_H$ is the Heaveside step function. Thus, replacing in Eq. (A2), the conductance becomes

$$G = (e^2/h) \sum_{\gamma} f(\varepsilon_{\gamma}, \varepsilon_F, T) = (e^2/h) \sum_{\gamma} \frac{1}{e^{(\varepsilon_{\gamma} - \varepsilon_F/k_B T)} + 1} \quad (\text{A4})$$

and the effective number of channels can be evaluated as the ratio

$$N_{ch} = \frac{G}{G_0}. \quad (\text{A5})$$

If the Fermi level vanishes ($\varepsilon_F=0$), for each metallic SWNT (or shell) the van Hove singularities are located at $\varepsilon_{\gamma}=(\hbar v_F m)/R$, while in the limit of large R the sum over γ can be replaced by an integral, so that

$$\begin{aligned} G &= G_0 \sum_m f(\varepsilon_m, 0, T) \sim G_0 \left[1 + 2 \int_0^{\infty} \frac{R d\varepsilon}{\hbar v_F} f(\varepsilon_m, 0, T) \right] \\ &= G_0 \left[1 + 2 \frac{R}{\hbar v_F} \ln(2) k_B T \right]. \end{aligned} \quad (\text{A6})$$

Here, 1 holds for the van Hove singularity for $m=0$, and the factor 2 includes the $\pm m$ symmetry.

APPENDIX B: CONTINUUM MODEL

1. FROM THE SUM TO THE INTEGRALS

Here, we discuss how the sums over the number of states, the number of shells and the number of subbands can be usefully replaced by integrals.

a. Linear part

The sum over n_y can be based on the relation $k_y = (2\pi n_y/2L_y)$ and $K_f = (2\pi N_f/2L_y)$. Thus, we can write

$$\sum_{n=0}^{N_f} \rightarrow \frac{2L_y}{2\pi} \int_0^{N_f} dk_y.$$

b. Radial part

The sum over shells for MWNT can be replaced by an integral on the radius. The transformation is based on the relation $R_{n_s} = R_i + \delta n_s$, thus the sum over n_s becomes

$$\sum_{n=0}^{N_s} \rightarrow \frac{1}{\delta} \int_{R_i}^{R_o} dR.$$

Thanks to the latter formula, we can evaluate

$$\begin{aligned} N_{ch} &\approx \sum_{n=0}^{N_s} N_{ch}(R_{n_s}) \sim b \int_{R_i}^{R_o} (aR + b) dR \\ &= \frac{R_o - R_i}{\delta} \left[\frac{a}{2} (R_o - R_i) + b \right], \end{aligned} \quad (B1)$$

which differs from the one obtained by using the sum

$$\begin{aligned} N_{ch} &= \sum_{n=0}^{(R_o - R_i/\delta)} N_{ch}(R_{n_s}) = \sum_{n=0}^{(R_o - R_i/\delta)} (aR_i + n\delta + b) \\ &= \left(1 + \frac{R_o - R_i}{\delta} \right) \left[\frac{a}{2} (R_o - R_i) + b \right]. \end{aligned} \quad (B2)$$

c. Angular part

Also the sum over m can be replaced by an integral; e.g., when we assume $\varepsilon_m = \hbar^2 m^2 / (2m^* R^2)$, we have

$$\sum_{m=0}^{M_f} \rightarrow \frac{\sqrt{2m^* R}}{\hbar} \int_0^{\varepsilon_f} \frac{d\varepsilon}{\sqrt{\varepsilon}}.$$

2. PERTURBATIVE SOLUTION FOR THE INTERTUBE TUNNELING

Let us assume $m \neq 0$, $\alpha_w = 0$, and $k_y = 0$ (we focus on the van Hove singularities). The general formula for the perturbative correction to the m , k_y , and R_{n_s} state is

$$\Delta \varepsilon_{m, k_y, R_{n_s}} \sim \sum_{n=1}^{N_s} (1 - \delta_{n, n_s}) \frac{U_{n, n_s}^2}{\varepsilon_{m, k_y, R_n} - \varepsilon_{m, k_y, R_{n_s}}}$$

and it can be written in terms of integrals. Here,

$$\begin{aligned} \varepsilon_{m, k_y, R_n} - \varepsilon_{m, k_y, R_{n_s}} &\sim v_F \hbar |m| \frac{R_{n_s} - R_n}{R_{n_s} R_n}; \\ U_{n, n_s} &= U_0 e^{-(|R_{n_s} - R_n|/W)} \end{aligned}$$

and we replace the sum with integrals

$$\begin{aligned} \Delta \varepsilon_{m, 0, R_{n_s}} &\sim \frac{U_0^2 R_s}{\delta v_F \hbar |m|} \left\{ \int_{R_i}^{R_s - \delta} \left[\frac{e^{-2(R_s - R)/W}}{R_s - R} \right] R dR \right. \\ &\quad \left. - \int_{R_s + \delta}^{R_o} \left[\frac{e^{-2(R - R_s)/W}}{R - R_s} \right] R dR \right\}, \end{aligned}$$

where $R = R_n$ and $R_s = R_{n_s}$.

According to Ref. 32 $U_0 \sim 100$ eV, $W \sim 2 \times 10^{-2}$ nm, and $\delta \sim 0.34$ nm.

$$\begin{aligned} \Delta \varepsilon_{m, 0, R_{n_s}} &\sim \frac{U_0^2 R_s}{\delta v_F \hbar |m|} \left\{ R_s \left[E_i \left(\frac{2x}{W} \right) \right]_{R_o - R_s}^{R_s - R_i} \right. \\ &\quad \left. + W [e^{-(2(R_s - R_i)/W)} + e^{-(2(R_o - R_s)/W)} - 2e^{-(2\delta/W)}] \right\}, \end{aligned} \quad (B3)$$

where $E_i(x)$ is the exponential integral, a special function defined on the complex plane. Since W is quite smaller than the other length parameters, we can expand $E_i(z)$ in series by obtaining

$$E_i(z) \sim \frac{e^z}{z}.$$

Thus, we get

$$\begin{aligned} \Delta \varepsilon_{m, 0, R_{n_s}} &= \frac{U_0^2}{|m| v_F \hbar R_s} \frac{W}{2\delta} \left\{ \left[-\frac{R_i e^{-(2(R_s - R_i)/W)}}{R_s - R_i} \right. \right. \\ &\quad \left. \left. - \frac{R_o e^{-(2(R_o - R_s)/W)}}{R_o - R_s} + \frac{2e^{-(2\delta/W)}(R_s - \delta)}{\delta} \right] \right\}. \end{aligned} \quad (B4)$$

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