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Conductance modulation of metallic carbon nanotubes by remote charged rings

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Abstract. – We calculate the effects of a longitudinal electrostatic perturbation on a metallic single-wall carbon nanotube and demonstrate conductance modulation. Such external modulation would be completely screened in bulk 3D metals but is possible in SWNTs because their electrons are quasi–two-dimensional and can interact with a nearby system of charges. The resultant modulation of the conductance is determined by the strength of the self-consistent potential and its periodicity over shorter or longer distances. We employ the zero-temperature single-particle Green's function transport approach in the empirical tight-binding approximation to quantify the modulation of conductance and also consider the limit of a superlattice.

Introduction. – The high quantum conductance of metallic Single-Wall Carbon Nanotubes (SWNTs), in the absence of defects or interconnects, is promising for applications. It has been demonstrated that vacancies, configurational defects [1,2] and mechanical deformations lower the conductance of a pristine tube. All-metallic SWNT circuits would have the best performance if one were able to modulate their conductance without recourse to structural modifications. SWNTs are cylinders created by rolling a graphene sheet; *i.e.*, quasi–two-dimensional (surface) entities, in contrast to 3D metallic systems. Therefore, a perturbation placed along a SWNT implemented —*e.g.*, by a molecule or surface potential with given periodicity [3]— will alter the electronic properties of an isolated tube. We propose in this letter some conditions that will lead to the modulation of conductance by the creation of local gaps in a metallic SWNT. We recently suggested the possibility of conductance modulation in metallic SWNTs by local gates [4], and have also been exploring symmetry properties that are involved in gap creation [5]. We consider a periodic oscillation of the self-consistent potential for the conduction electrons along the length of an infinite SWNT and a perturbation of a finite section of the tube that also shows similar conductance modulation. The three

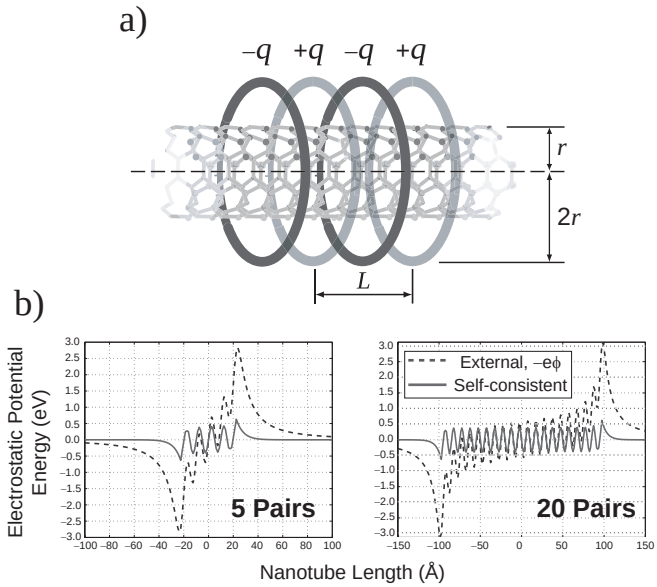

Fig. 1 – a) A metallic, [5, 5] SWNT placed in an electrostatic potential $\phi(\boldsymbol{r})$ originating from axial-symmetric rings of radius $2r$, where r is the SWNT radius. A charge of magnitude $|q|$ alternating in sign is placed on consecutive rings. b) The change in potential energy, $-e\phi(\boldsymbol{r})$, caused by the external rings alone (dashed line) and the resulting potential energy after self-consistent rearrangement of π-electrons (within Hartree-Fock theory), for 5 pairs (left) and 20 pairs (right) of rings, using $|q| = 2.5e$. Twice the distance between equally spaced rings defines the superlattice length L which here is four times the SWNT lattice constant, $L = 4L_0$. $L_0 = \sqrt{3}a$ and $a = 1.44$ Å is the distance between nearest carbon atoms.

factors involved are:
1) The strength of the self-consistent-potential induced by the remote charges.
2) The length of the unit cell of the superlattice.
3) The total number of unit cells of the superlattice that are in proximity to the SWNT.

Model and methods. – We consider a neutral SWNT and focus on the perturbation caused by excess charges alternating in sign, placed onto equally spaced rings. The charge is uniformly distributed on a given ring of radius $2r$, where r is the SWNT radius (fig. 1(a)). A typical magnitude of the excess charge we use is $|q| = 2.5e$. We choose an axially symmetric potential to model the effect caused by the variation of the potential along the SWNT. The resultant redistribution of the π-electrons caused by the external potential $\phi(\boldsymbol{r})$ induces an electrostatic Coulomb potential that counteracts the external potential. As one can see in fig. 1(b), the self-consistent potential oscillates within the gated region and exhibits long tail-ends. The total self-consistent potential is naturally more uniform than the external potential $\phi(\boldsymbol{r})$ given by the dashed line in fig. 1(b). However, the screening is far from complete. This oscillation period plays a crucial role for the modulation of conductance. We employ and combine single-particle Green's functions, a modified tight-binding Hamiltonian and also use the Kronig-Penney model to capture the elementary physics involved in the conductance modulation. We account for the effect of charge redistribution [6] within the Hartree-Fock approximation assuming charge equilibrium for the remote rings. The π-electrons that are responsible for electron transport are modelled by using the empirical nearest-neighbor tight-

binding approach [7]:

$$\langle \boldsymbol{r}|\Psi_{n_0}\rangle = \sum_i C^i_{n_0}\Phi_\pi(\boldsymbol{r}-\boldsymbol{r}_i). \tag{1}$$

Here $\{\boldsymbol{r}_i\}$ represent the positions of the SWNT carbon atoms. $\Phi_\pi(\boldsymbol{r}-\boldsymbol{r}_i)$ are atomic orbitals for the π-electrons. The nearest-neighbor tight-binding approximation reproduces the characteristics of π-electrons fairly well. The Hamiltonian in this approximation is given by

$$\hat{H}_0 = \sum_{\langle ij\rangle}\gamma_\pi \hat{c}^\dagger_i \hat{c}_j\,, \tag{2}$$

where $\gamma_\pi = -2.7\,\mathrm{eV}$ is the hopping integral [7], and $\langle ij\rangle$ indicates that the sum is performed only for neighboring sites i and j. The coefficients $C^i_{n_0}$ are determined by the eigenvectors $|\Psi_{n0}\rangle$ of H_0 according to (1). (We sort the eigenvectors in order of their energy levels E_{n_0}.) However, because charge neutrality is locally violated, one must modify the Hamiltonian (2) and we follow a procedure described in [6]. For our basis, the Coulomb kernel is

$$U_{ij,kl} = \delta_{ij}\delta_{kl}\times\begin{cases}\frac{1}{r_{ik}}\,, & i\neq k,\\ U_0\ (\text{in our units, } eU_0 = 14.6\,\mathrm{V}), & i=k\end{cases} \tag{3}$$

($r_{ik} = |\boldsymbol{r}_i - \boldsymbol{r}_k|$). For our perturbation —an external potential energy of magnitude $-e\phi(\boldsymbol{r})$— the SWNT as a whole remains neutral (the total number of π-electrons for a given spin n_{CN} is well defined once the length of the SWNT to be modeled has been chosen), but a local redistribution of charge occurs. We assume that the charge distribution of the remaining atomic electrons (both core and σ-electrons which we refer to as background charge) is not modified by the external field, which holds provided the field is small. Then the relative change of the charge with respect to the unperturbed tube is related to the density matrix:

$$\delta\rho_{ij} = -2e\left[\sum_{n=1}^{n_{CN}}\langle\boldsymbol{r}_i|\Psi_n\rangle\langle\Psi_n|\boldsymbol{r}_j\rangle - \sum_{n_0=1}^{n_{CN}}\langle\boldsymbol{r}_i|\Psi_{n_0}\rangle\langle\Psi_{n_0}|\boldsymbol{r}_j\rangle\right] = -2e\left[\sum_{n=1}^{n_{CN}}C^i_n\big(C^j_n\big)^* - \sum_{n_0=1}^{n_{CN}}C^i_{n_0}\big(C^j_{n_0}\big)^*\right].$$

We now calculate both $\delta\rho_{ij}$ and $\{|\Psi_n\rangle\}$ self-consistently within the Hartree-Fock approximation as a solution of the following Hamiltonian (Einstein's summation rule implied):

$$\hat{H} = \hat{H}_0 + \left(-e\phi_e(i)\delta_{i,j} + eU^{\mathrm{HF}}_{ij,kl}\delta\rho_{kl}\right)\hat{c}^\dagger_i\hat{c}_j\,, \tag{4}$$

where

$$eU^{\mathrm{HF}}_{ij,kl}\delta\rho_{kl} = e\left(U_{ij,kl} - \frac{1}{2}U_{il,kj}\right)\delta\rho_{kl} = \sum_{i\neq k}\delta_{ij}e\frac{\delta\rho_{k,k}}{r_{ik}} - \frac{e}{2}\frac{\delta\rho_{ij}}{r_{ij}}\,.$$

In the previous equation, the term $-e\delta\rho_{ij}/2r_{ij}$ runs for $j\neq i$. For $-e\phi(\boldsymbol{r}_j)\to 0$ the positive and negative charges balance and $\delta\rho_{ij}\to 0$. This reduces the Hamiltonian (4) to the familiar case, (2).

For $\phi(\boldsymbol{r})$ produced by a periodic arrangement of rings (fig. 1(a)), the self-consistent potential energy exhibits a few oscillations with period L equal to twice the spacing between rings. We consider here a [5, 5] nanotube. However, the following argument applies to *any* metallic SWNT, provided modifications to the dispersion relation and analytical Green's functions are made.

The eigenvalues of H_0 for an unperturbed [5, 5] SWNT are given by [7]

$$E_{s,0}(k,m) = s\gamma_\pi\sqrt{1+4\cos\left(\frac{\sqrt{3}}{2}ka\right)\left[\cos\left(\frac{\sqrt{3}}{2}ka\right)+\cos\left(\frac{\pi m}{5}\right)\right]}\,, \tag{5}$$

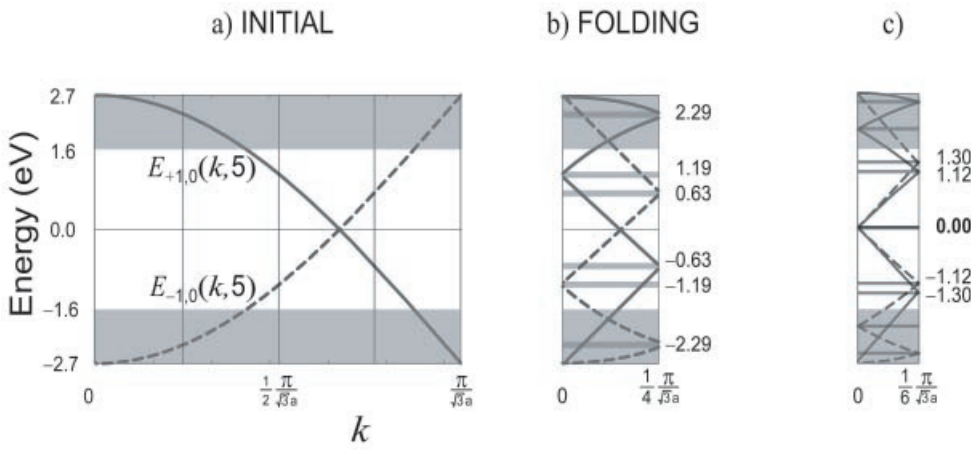

Fig. 2 – a) Dispersion relation for the two bands ($E_{+5,0}, E_{-5,0}$) crossing at the Fermi level ($E = 0$) for a $[5, 5]$ SWNT. A small, periodic perturbation along the SWNT will cause, according to the Kronig-Penney model, forbidden gaps for electronic motion at the regions where folding occurs. b) For a field with the periodicity given in fig. 1, folding would occur at the energies shown. c) For comparison purposes, we also show the dispersion relation for a superlattice length L equal to $6L_0$. A $[5, 5]$ SWNT placed in this superlattice would become a semiconductor.

where k is the wave vector along the length of the SWNT, m is the (quantized) circumferential wave vector and $s = \pm 1$ (sometimes referred to as "pseudospin") arises from orthogonality of the two wave functions belonging to different sublattices for the hexagonal lattice. For the $E_{s,0}(k, 5)$ bands, which are the most important for transport, we need to modify eq. (5) so that the energies are monotonic functions of k. We depict them in fig. 2(a), which shows the two bands present close to the Fermi level. There are more bands present in the gray zone, but they are not displayed because they are not relevant for the discussion. For this region, conductance is equal to $2G_0$, where $G_0 = \frac{2e^2}{h}$ is the quantum of conductance.

Consider first an infinitely long SWNT embedded in a superlattice created by an infinite array of equally spaced rings. The self-consistent potential would then be periodically oscillating and this would induce, according to the Kronig-Penney model, a folding of the bands. We show the effect in the dispersion relation in fig. 2. Vertical lines in fig. 2(a) indicate the zone folding as a result of a perturbation which decreases the size of the Brillouin zone by a factor of four. In fig. 2(b) we show the modified band structure. Bold horizontal lines show forbidden energy regions for the electrons of a given band. Since there are two bands and folding does not occur simultaneously for both of them for the same value of energy, we expect in this case the conductance to be lowered at most by $1G_0$. The reason for this modulation is that for a vicinity of the k-points where folding occurs, a mini-gap develops. This gap-opening is equivalent to a lowering of the density of states (DOS), and this suppression of the DOS results in the modulation of the conductance. For large enough $|V|$ ($|V|$ is the strength of the self-consistent potential), an overlap of two gaps and further suppression of the conductance becomes possible. Also, a perturbation with periodicity that equals a multiple of $3L_0$ will fold the bands at the Fermi point, where the two bands cross: We show the modified band structure for a self-consistent potential with periodicity $6L_0$, $\sim 1.5\,\text{nm}$ in fig. 2(c). Such a perturbation will create a gap for both bands and, as a result, the conductance at the Fermi point will be zero.

Previous argument can be applied when the length of the CNT unit lattice (L_0) is commensurate with twice the spacing between rings (L): $nL_0 = mL$ for n and m integers. The Kronig-Penney model cannot be used if the periods of the CNT lattice and the lattice for the rings are incommensurate. For a finite system, we believe that even an incommensurate potential will alter the dispersion of the CNT charge carriers in certain regions in k-space corresponding to the Fourier component of the potential. This translates into conductance modulation at certain values of energy. Since a strong modulation of conductance requires a long section in which the local density of states is suppressed, one must consider a finite-length potential that is long enough or strong enough. This indicates the relation between the modulating effect and the size of the unit cell for the superlattice.

We now describe the effects of a small number of rings around a metallic SWNT. We use the approach of Datta [8] to calculate the electron transport properties. We obtain the relative decrease in conductance in the [5, 5] SWNT in terms of zero-temperature single-particle Green's functions. The Green's function we use is

$$G^R(E) = \left[H - E \times I + \Sigma_L(E) + \Sigma_R(E)\right]^{-1}, \tag{6}$$

where H is defined by eq. (4) and

$$\begin{aligned}
\Sigma_L(E) &\equiv -H_{CL} G^R_{LL}(E) \left[I_{LL} - H_{LC} G^R_{CL}(E)\right]^{-1} H_{LC}\,, \\
\Sigma_R(E) &\equiv -H_{CR} G^R_{RR}(E) \left[I_{RR} - H_{LC} G^R_{CR}(E)\right]^{-1} H_{RC}\,.
\end{aligned}$$

H_{CL} and H_{CR} are the submatrices in the Hamiltonian connecting the section under study (C) and semi-infinite, unperturbed sections of the [5, 5] SWNT at its left (L) and right (R) (which we call hereafter "leads"). $H_{LC} = H^T_{CL}$ and $H_{RC} = H^T_{CR}$. For the [5, 5] SWNT, $\Sigma_{L,R}$ are nonzero only for the submatrices of dimensions 10×10 which are located at the positions where our finite tube is in contact with the leads. G^R_{LL}, G^R_{RR}, G^R_{CL} as well as G^R_{CR} are also 10×10 matrices. Further symmetry for the [5, 5] SWNT allows to have orthogonal wave functions within a unit cell having two carbon atoms. This allows one to obtain the aforementioned G^R-submatrices in terms of the 2×2 matrix:

$$G^R\big((p,q),(p',q');E\big) = \frac{\sqrt{3}a}{10\pi} \sum_{m=-4}^{5} \int_{-\frac{\pi}{\sqrt{3}a}}^{\frac{\pi}{\sqrt{3}a}} M(k,m) \exp\left[i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')\right] \mathrm{d}k, \tag{7}$$

where the matrix $M(k,m)$ carries the information required by orthogonality of wave functions in a unit cell having two atoms:

$$M(k,m) \equiv \begin{pmatrix} \frac{1}{E_{-1,0}(k,m)-E+i\eta} + \frac{1}{E_{+1,0}(k,m)-E+i\eta} & \frac{e^{-i\theta(k,m)}}{E_{-1,0}(k,m)-E+i\eta} - \frac{e^{-i\theta(k,m)}}{E_{+1,0}(k,m)-E+i\eta} \\ \frac{e^{i\theta(k,m)}}{E_{-1,0}(k,m)-E+i\eta} - \frac{e^{i\theta(k,m)}}{E_{+1,0}(k,m)-E+i\eta} & \frac{1}{E_{-1,0}(k,m)-E+i\eta} + \frac{1}{E_{+1,0}(k,m)-E+i\eta} \end{pmatrix}, \tag{8}$$

$\eta \to 0^+$, the eigenenergies $E_{s,0}(k,m)$ are given by eq. (5),

$$\begin{aligned}
\phi_q(p) &\in \begin{cases} \left\{0, \frac{2\pi}{5}, \frac{4\pi}{5}, \frac{6\pi}{5}, \frac{8\pi}{5}\right\} & \text{for odd } p, \\ \left\{\frac{\pi}{5}, \frac{3\pi}{5}, \pi, \frac{7\pi}{5}, \frac{9\pi}{5}\right\} & \text{for even } p, \end{cases} \\
e^{i\theta(k,m)} &= \frac{2e^{\frac{m\pi i}{5}} \cos\left(\frac{\sqrt{3}}{2}ka\right) + 1}{\sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2}ka\right)\left[\cos\left(\frac{\sqrt{3}}{2}ka\right) + \cos\left(\frac{\pi m}{5}\right)\right]}},
\end{aligned}$$

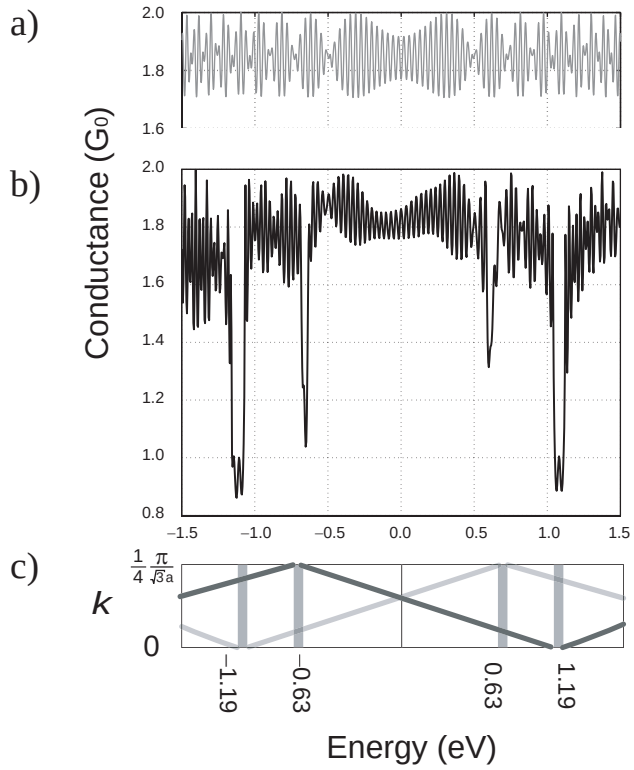

Fig. 3 – a) Conductance as obtained with our method for an unperturbed [5, 5] SWNT of length $\sim 50\,\mathrm{nm}$. b) Modulation of conductance for 50 pairs of rings, $|q| = 2.5e$ and spacing between rings given in fig. 1. c) Dip positions agree with values predicted by the Kronig-Penney model. Besides additional interference, only one conduction channel is at most suppressed.

and the factor

$$\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}') = \sqrt{3}(p-p')\frac{ka}{2} + m\big(\phi_q(p) - \phi_{q'}(p')\big)$$

gives the phase relations for electrons to propagate between different unit cells. For the Green's functions we are concerned about, we have $p = 0, \pm 1$.

Although this scheme has been used to calculate electronic transport in semiconducting SWNTs, to our knowledge this is the first instance in which an analytical Green's function is explicitly presented for a nanotube. Finally, we calculate the transmittance T (and hence ballistic conductance $G(E) = G_0 T(E)$) as

$$T(E) = Tr\left[\Gamma_L G^{R\dagger}(E)\Gamma_R G^R(E)\right], \tag{9}$$

with the additional identification [8] $\Gamma_{L,R}(E) = 2\,\mathrm{Im}\,\Sigma_{L,R}(E)$.

Results and conclusions. – In fig. 3(b) we show the conductance modulation for 50 pairs of rings as those shown in fig. 1(a). They correspond to a unit lattice of length $4L_0$. The self-consistent potential is caused by a charge $|q| = 2.5e$ on each ring and applied to a [5, 5] SWNT of length $200L_0$. A significant suppression of the conductance can be seen at four values of energy which are determined by the energies at which band-folding occurs. These

have been given in fig. 2(b) and are shown for comparison in fig. 3(c). They clearly agree even though now the perturbation is of finite length. For an unperturbed [5, 5] SWNT, the conductance in this energy range is equal to $2G_0$, since there are two conduction channels present (fig. 3(a)). In our results, the transmission varied from 2 to 1.8 and shows a number of low-amplitude dips and heights in the transmittance that increases linearly with the length of the SWNT. Because the goal of our work is to investigate the major suppression of the conductance due to the periodic self-consistent potential, we did not further investigate this low-amplitude structure or attempt to remove it by thermal averaging.

A clear suppression of conductance at the energy points calculated within the Kronig-Penney model can be seen. Unlike the case of heterojunctions created by nanotubes of different chiralities, in this case there is no mismatch between the quantized component of the wave vector. This means that the conductance is high and close to the nominal value $2G_0$ for energy regions apart from the folding energies. We finally mention that we have observed in our calculations a logarithmic dependence between the length to which the perturbation is applied (for fixed external potential) and conductance, and similarly a logarithmic dependence between conductance modulation and the magnitude of q (for a fixed length).

In conclusion, we have shown the possibility of conductance modulation in metallic SWNTs by applying a longitudinal periodic electrostatic perturbation along a section of finite size. We remark the fact that if any metallic tube (independent of its actual chirality) is being placed in the proximity of a structure as the one we have described, its conductance can be modulated. Furthermore, since the electrostatic potential that we consider does not have any components along the circumference, no mismatch between wave functions in the gated region and the free tube arises, as is usually the case for metall-semiconducting junctions. This keeps the value of the conductance close to that of a free, ballistic, metallic SWNT in regions comprising energies other than the ones where bending occurs.

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