Violation of the single-parameter scaling hypothesis in disordered graphene nanoribbons

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A numerical statistical analysis of the conductance g distribution function in disordered graphene nanoribbons is presented. Calculations are performed within the nonequilibrium Green's Function formalism. We have checked that the conductance variance in these quasi one-dimensional systems scales linearly with the average of the logarithm of g, i.e., $\sigma^2 = A < -\ln g > + B$ in the localization regime. However, the slope A is not a constant as the disorder degree varies in any region of the energy spectrum, i.e., the single parameters scaling hypothesis is not verified. Our results stimulate further investigations in order to categorize the conductance fluctuations on the basis of the band structure and/or lattice topology of the system in study.

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The single parameter scaling (SPS) hypothesis[1] for the distribution function $\wp(g)$ of the conductance g in disordered systems has received in the last decade a systematic assessing in one-dimensional (1D) (Refs. 2 and 3) and higher dimensionality systems[4,5] by means of analytical and numerical investigations. These works have established that $\wp(g)$ is a universal function, characterized by a single scaling length (i.e., the localization length ξ), in a wide region of the energy spectrum away from the band tails. This important statement has been verified not only in 1D (Ref. 2) systems but also in some two-dimensional (2D) and three-dimensional (3D) models of disordered materials.[5] Although these results represent fundamental advancements in the field of localization theories, they could be hardly validated by means of experimental analysis in real systems, mainly due to difficulties in the fabrication of nearly ideal nanostructures with a refined control of the geometry (e.g., shape, size, etc.) and the disorder status.

Recently single graphene sheets have been synthesized, e.g., by chemical exfoliation of graphite[6] or through thermal decomposition of SiC.[7] The availability of this unique material has opened new perspectives to explore quantum transport in low-dimensional carbon-based systems, eventually investigating also disorder effects. Indeed, graphene nanodevices, e.g., based on quasi-1D graphene nanoribbons (GNRs),[8] seem ideally suited for experiments on the conductance distribution. As a consequence the results related to the SPS hypothesis could, in principle, be also verified. However, due to its peculiar electronic properties (including linear dispersion and electron-hole symmetry) the transport features of disordered graphene-based conductors could be unconventional, and the achieved categorization could be invalid for such structures.

In this work we have investigated the localization issue in strongly disordered GNRs in the framework of the Anderson model using the nonequilibrium Green's Function (NEGF) techniques. Our numerical results show systematic deviations (i.e., for the entire energy spectrum) from the SPS for the conductance distribution in these systems.

We use the Anderson Hamiltonian (AH) as a model of the disordered graphene nanoribbons. The model[9] reads

$$H = -t_0 \sum_{\langle n,l\rangle,\sigma} c^+_{n,\sigma} c_{l,\sigma} + c^+_{l,\sigma} c_{n,\sigma} + \sum_{n,\sigma} \varepsilon_n c^+_{n,\sigma} c_{n,\sigma}. \quad (1)$$

Here the symbol $\langle n,l\rangle$ indicates that the sum runs on next neighbor sites of the graphene honeycomb lattice. $c^+_{n,\sigma}(c_{n,\sigma})$ is the creation (annihilation) operator of an electron with spin σ at the site n, $t_0 = 2.7$ eV (Ref. 10) is the hopping integral between two next neighbor carbons atoms, and ε_n is the site n energy. The value of ε_n / t_0 has been chosen randomly in the interval $(-W/2, W/2)$. We have considered armchair graphene nanoribbons (AGNRs) and zigzag graphene nanoribbons (ZGNRs), which are classified using the convention of Ref. 10, i.e., with the integers N_a and N_z indicating, respectively, the number of dimer lines and zigzag chains across the ribbon width. The system length L is also indicated by an integer which is the number of atoms belonging to the dimer lines (for the AGNRs) and zigzag chains (for the ZGNRs).

The NEGF formalism is applied to calculate the zero-temperature conductance $g(E) = (2e^2/h)T(E)$ (which in the following will be reported in $2e^2/h$ units) at the Fermi energy E, where T is the transmission coefficient $T = \mathrm{Tr}[\Gamma_L G \Gamma_R G^\dagger]$. The NEGF is $G = (E^+ I - H - \Sigma_L - \Sigma_R)$, where I *is* the identity operator, Σ_L, Σ_R are the self-energies including the effect of scattering due to the left (L) and right (R) contacts, and the contact spectral functions are $\Gamma_{L,R} = i(\Sigma_{L,R} - \Sigma^+_{L,R})$. The contact self-energy can be expressed as $\Sigma = \tau g_s \tau^\dagger$, where g_s is the surface Green's function of the lead and τ is the interaction between the conductor and the contact.[11] For the leads we consider two semi-infinite ribbons of the same width N_a or N_z as the conductor, represented by the same Hamiltonian without diagonal disorder. An optimized recursive technique allows performing our numerical

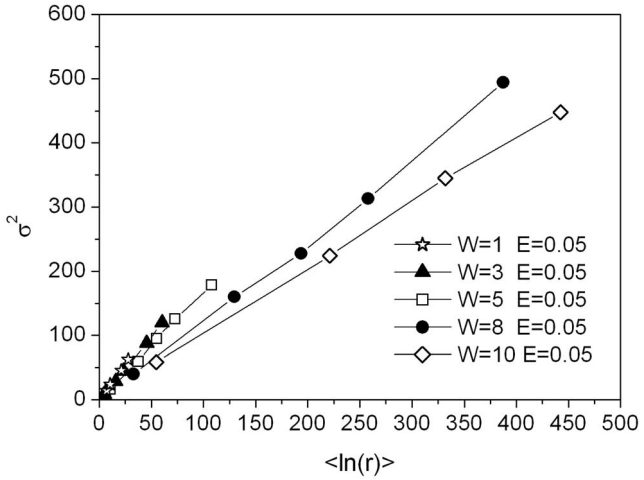

FIG. 1. Conductance fluctuations σ^2 as a function of $\langle \ln(r) \rangle$ for $E=0.05$ eV Fermi energy and for different values of the disorder in the case of ZGNRs with width $N_z=50$.

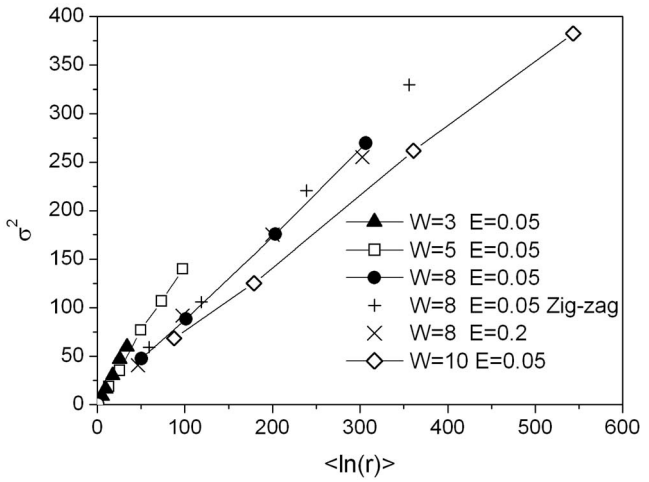

FIG. 2. Conductance fluctuations σ^2 as a function of $\langle \ln(r) \rangle$ for $E=0.05$ eV Fermi energy and for different values of the disorder in the case of AGNRs with width $N_a=200$. In the case of $W=8$ results are shown also for ZGNRs with $N_z=100$ and for AGNRs with $N_a=200$ and $E=0.2$ eV.

analysis in very large systems reducing by a factor of L the size of the matrix to be inverted.[12]

As we could expect, our numerical analysis has established that in the localized regime the average zero-temperature resistance $r(E)=g(E)^{-1}$ of both AGNRs and ZGNRs depends exponentially on L, therefore,

$$\langle \ln r(E) \rangle = 2L/\xi + c, \tag{2}$$

where c is a small constant, which does not depend on the Fermi energy, as E is not in the tails of the spectrum. In 1D systems also the variance of the logarithm of the zero-temperature conductance

$$\sigma^2 = \langle \ln^2 g \rangle - \langle \ln g \rangle^2 \tag{3}$$

is proportional to the conductor length. Moreover SPS states that this dependence of σ^2 is ruled only by the localization length. In the 2D case, recent works[13] on square-lattice-based systems have validated SPS while demonstrating a power-law dependence on L/ξ, i.e., $\sigma^2 \propto (L/\xi)^{2/3}$. GNRs are quasi-1D systems with a honeycomb structure, and in principle, different scaling behaviors can be expected with respect to those reported in the previous works. In Fig. 1 σ^2 is shown as a function of $\langle \ln r(E) \rangle$ (and implicitly as a function of $2L/\xi$) for ZGNRs with a width $N_z=50$ and a Fermi energy of $E=0.05$ eV. Each point represents a statistical analysis on more than 10^3 replicas of the studied systems. In the figure the value of the disorder W is indicated. A similar analysis is shown in Fig. 2 for AGNRs with width $N_a=200$ and the same Fermi energy. In Fig. 2, for the $W=8$ case, we also show the σ^2 dependence on $\langle \ln r(E) \rangle$ for AGNRs with $N_a=200$ and $E=0.2$ eV, and for ZGNRs with width $N_z=100$ and $E=0.05$ eV. The latter results do not show significant differences with respect to the case of AGNRs with $N_a=200$ and $E=0.05$ eV.

Our statistical analysis indicates that a linear dependence

$$\sigma^2 = A\langle \ln r(E) \rangle + B \tag{4}$$

properly describes the conductance fluctuation of disordered GNRs (of course σ^2 is also linear on $2L/\xi$). Therefore, in this sense they resemble the behavior of a pure 1D system. However, SPS also implies that A must be independent of the disorder parameter W; but, as it can be easily inferred from Figs. 1 and 2, our results strongly deviate from this statement.

A critical analysis of the SPS hypothesis in 1D model Hamiltonians with and without correlated disorder has been reported in a series of works.[2,14] The main interest was quantifying the rules for the SPS validity in the critical tail regions of the spectra. These papers, based also on analytic results, suggest a criterion for the validity of the SPS; i.e., the SPS is essentially controlled by another length scale $l_2(E)$ related to the density of states (DOS), which in the case of a single band, has the following expression:

$$l_2(E) = \sin[\pi N(E)/N_{\text{tot}}]^{-1}, \tag{5}$$

where the integrated DOS $N(E)$ and the total density N_{tot} are given by

$$N(E) = \int_{-\infty}^{E} \text{DOS}(E)dE, \quad N_{\text{tot}} = \int_{-\infty}^{+\infty} \text{DOS}(E)dE. \tag{6}$$

The parameter $l_2(E)$ gets its minimum value ~ 1 at half filling, while it is very large in the band tails, and the inequality $l_2(E) > \xi(E)$ determines the region of the spectrum where the SPS does not hold. Numerical results based on the AH in a square lattice show that this rule is correct also for systems with higher dimensionality; however, the contiguity of the hole band and electron band at $E=0$ in graphene poses some doubts on straightforward extensions of expressions (5) and (6) for the $l_2(E)$ evaluation in the GNR case. As a first attempt we can assume that there is a continuity of the spectrum at $E=0$; therefore, when E is small $l_2(E)$ gets values

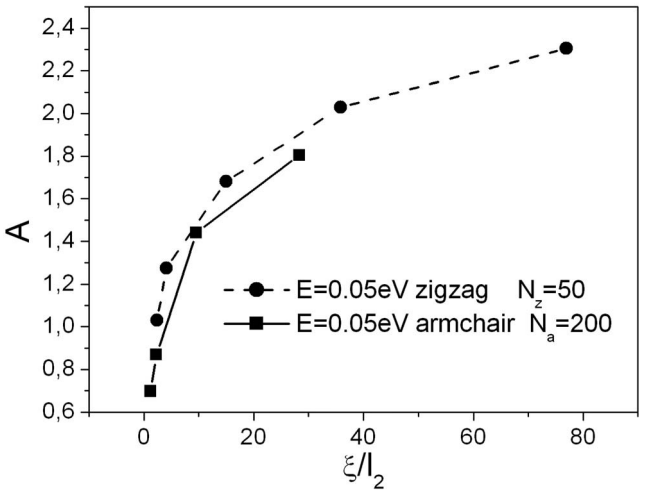

FIG. 3. Slope A of the conductance fluctuations $\sigma^2 = A\langle \ln r(E)\rangle + B$ as a function of the ξ/l_2 ratio for the indicated structures and energies.

similar to those obtained for the half-filled band case [i.e., one electron per orbital $N(E) \sim N_{\text{tot}}/2$]. Following this assumption we have calculated (Fig. 3) the A values in Eq. (4) as a function of ξ/l_2 using the results reported in Figs. 1 and 2. According to the SPS validity criterion we should expect a strong dependence of A on ξ/l_2 only when $\xi/l_2 < 1$ and a plateau for $\xi/l_2 > 1$ (see a similar analysis in Ref. 13). This is clearly not the case for both the AGNR and ZGNR systems considered.

One could argue that the $E=0$ point (i.e., the Dirac point of the corresponding graphene system) is an effective tail region of the energy spectrum since the hole ($E<0$) and electron ($E>0$) bands should be considered as two separate bands in the $l_2(E)$ estimate (i.e., discontinuity hypothesis at the $E=0$) and $l_2(E \sim 0) \gg 1$. In order to explain the center of band anomaly in the 1D Anderson model, it is has been argued that $E=0$ can be considered as a band boundary also in the 1D case.[15] This argument would categorize our results

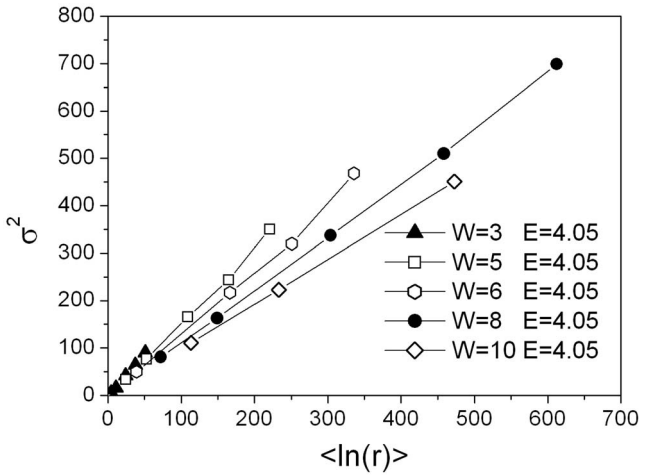

FIG. 4. Conductance fluctuations σ^2 as a function of $\langle \ln(r)\rangle$ for the Fermi energy $E=4.05$ eV and for different values of the disorder in the case of ZGNRs with width $N_z=50$.

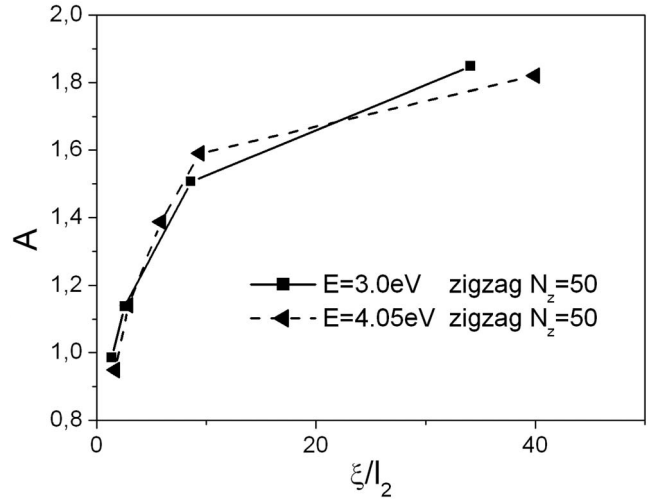

FIG. 5. Slope A of the conductance fluctuations $\sigma^2 = A\langle \ln r(E)\rangle + B$ as a function of the ξ/l_2 ratio for the indicated structures and energies.

on disordered GNR near the $E=0$ (Figs. 1 and 2), i.e., the violation of SPS, according to the cited criterion. In this case, e.g., for the electron band ($E>0$), we should indeed replace the expression in Eq. (6) with the following ones:

$$N(E) = \int_{E=0}^{E} \text{DOS}(E)dE, \quad N_{\text{tot}} = \int_{E=0}^{+\infty} \text{DOS}(E)dE. \quad (7)$$

As a consequence we should expect that $l_2(E)$ gets smaller when we move the Fermi energy well inside the electron (hole) band. In Fig. 4 σ^2 is shown as a function of $\langle \ln\ r(E)\rangle$ for ZGNRs with width $N_z=50$ with a Fermi energy of $E=4.05$ eV. Again, each point represents a statistical analysis on more than 10^3 replicas of the systems. A violation of the SPS hypothesis seems to emerge also from this statistical analysis. In order to confirm the difficulty to find any regime of the Fermi level where the SPS hypothesis is verified, A as a function of ξ/l_2 is shown in Fig. 5 for ZGNRs with width $N_z=50$ and different values of E. Here l_2 is numerically evaluated[15] according to expressions (7) (i.e., considering $E=0$ as a band boundary). For none of the E values considered an evident plateau of A can be recovered; and, anyhow, A strongly varies when $\xi/l_2 > 1$.

The numerical analysis here presented indicates that the current knowledge in the field of the localization theory is not complete. Indeed, while literature results indicate a precise categorization for the validity of the SPS and the universality of $\wp(g)$ in terms of the global length parameters l_2 related to the energy spectra, our study demonstrates that the generalization of this criterion to any band structure and/or system lattice topology is critical. Further investigations are needed in order to find more appropriate categorization criteria. Moreover, the possibility to build GNR-based devices could stimulate experimental tests of such results by means of conductance measurements at very low temperatures.

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