



Theoretical Investigation on Transportance for Single-Walled Nanotubes and Bi-Layer Graphene

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ABSTRACT

The transport properties of several carbon nanoparticle derivatives, including single-layer nanotubes and bi-layer graphene, under an external constant electric field, are investigated. Results were analyzed and identified as a function of the quasi-classical approximation of relaxation time by using the Boltzmann kinetic equations. These approaches have been used to obtain the relationships between the electric conductivity $\sigma(E)$ and electrons diffusion coefficient $D(E)$ in carbon nanostructures. This study proves that when the temperature rises the electrical conductivity $\sigma(E)$ decreases for both single-layer and bi-layer carbon nanostructures. For a wide range of temperatures, the electrical conductivity $\sigma(E)$ behavior of the studied nanoparticles is nonlinearly dependent on the magnitude of the external electric field (E). In contrast, the electron diffusion coefficient $D(E)$ is independent of temperature for both single- and bi-layers. It also shows that the intensity of an external electric field possesses a nonlinear influence on the electron diffusion coefficient.

Keywords: single-walled nanotubes, bi-layer graphene, electrical conductivity, electron diffusion, Boltzmann kinetic equations.

INTRODUCTION

Carbon is one of the most significant and often occurring elements in nature, and it exhibits a range of ways of existence. Carbon is unique in that it can simultaneously exist in a number of crystalline forms, such as diamond, quasi-two-dimensional graphene, quasi-one-dimensional carbon, and quasi-zero-dimensional fullerenes. Numerous variations of carbon have only lately been found. Carbon nanotubes (CNTs) are extended cylindrical low-dimensional structures with a diameter ranging from one to several tens of nanometers and a length of up to several centimeters (Eletsky, 2007), consisting of one or more graphene sheets rolled into a tube and usually ending in a hemispherical head, which can be considered as half the molecule of fullerene. One atomic layer of graphite based on a hexagonal network of sp^2 -hybridized carbon atoms makes up the low-dimensional carbon structure known as graphene (Baimova and Rysaeva, 2015). Due to its distinct electrical characteristics, graphene is intriguing from both the standpoint of potential practical applications and from a theoretical perspective. Graphene's valence and conduction bands do not have an energy gap, electrons close to the Fermi level exhibit linear dispersion (Shahil *et al.*, 2012) (Lozovik and Sokolik, 2008). Low-dimensional carbon derivatives can be used as parts of various devices such as: diodes, transistors, logic components, switches, electrodes, sensors, atomic force microscopes (AFM), and scanning tunnelling microscopes (STM) (Cantalini and Valentinia, 2004). This is possible because low-dimensional carbon derivatives are versatile materials. Currently, there is an urge demand for researching the electrophysical characteristics of these derivatives because of their desirable traits in industrial applications. These derivatives have also a high potential to be used in chemistry, medicine, and biotechnologies (Harris, 2004). In this research, the focus is on investigating how the temperature affects the electrical transport characteristics of quasi-one-dimensional and quasi-two-dimensional of carbon derivatives involving, single-layer carbon nanotubes and bi-layer graphene ribbons.

Model and Effective Equations

The electrical properties of CNTs and how they influence by an external electromagnetic field are pivotal joint for numerous publications (Harris, 2004) (Mintmire and White, 1995). A model that considers only the π -electrons of the nearest neighboring atoms makes it possible to obtain a correct description of the main electronic properties of CNTs. The dispersion, which defines the electrical characteristics of graphene, is known as: (Lakhtakia, 2004):

$$E(p) = \pm \gamma \sqrt{1 + 4 \cos(ap_x) \cos\left(\frac{ap_y}{\sqrt{3}}\right) + 4 \cos^2\left(\frac{ap_y}{\sqrt{3}}\right)}, \quad \dots\dots\dots (1)$$

$$a = \frac{3b}{2\hbar},$$

Where

$E(p)$ – energy of π -electrons in the conduction and the valence bands, $\hbar$ -Planck constant, $p = (p_x, p_y)$, $\gamma = 2.68$ eV are the integrals of electron hopping element between adjacent crystal lattice sites, and the distance between nearby carbon atom is $b = 0.141$ nm in graphene. The conduction band and the valence band are denoted by various signs in the dispersion relation, respectively. It is possible to derive the CNT dispersion relation, if we consider how the graphene sheet is rolled into a cylinder and apply the conditions for quantization of the quasi-momentum P along the CNT circumference. We take into consideration single-walled CNTs $(n, 0)$ of the "zig-zag" form, which have semiconductor characteristics, likewise a quasi-one-dimensional carbon nanostructure (Dragoman, 2014). The problem geometry is shown in Fig. (1).

The dispersion relation for CNTs $(n, 0)$ of the "zig-zag" can be written as: (Lakhtakia, 2004):

$$E(p) = \pm \gamma \sqrt{1 + 4 \cos(ap_x) \cos\left(\frac{\pi s}{n}\right) + 4 \cos^2\left(\frac{\pi s}{n}\right)}, \quad \dots\dots\dots (2)$$

Where $s=1, 2, \dots, n$ – the components of momentums throughout the circumference of the nanotube, and $p=(p_x, s)$ is the quasi momentum of CNTs electrons.

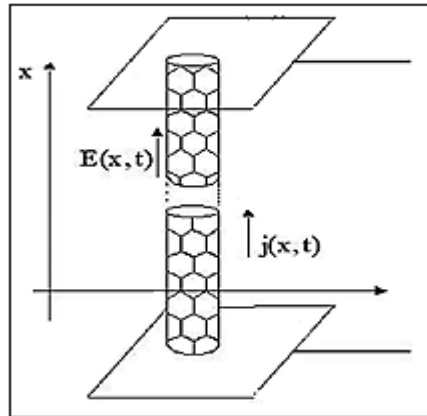


Fig. 1: CNTs of the "zigzag" type in an external electric field. The field strength vector E is directed along the CNT axis

The procedure of determining the electron transport coefficient in CNTs is sufficiently detailed in (Salimath and Ghosh, 2014) (Buligin *et al.*, 1999). The semiclassical relaxation time approximation is used to simulate the evolution of the electrical system. In the τ -approach, the Boltzmann kinetic equation yields the function of the electron distributions in a momentum state $p = (p_x, s)$ (Pitaevskii and Lifshitz, 1981):

$$\frac{\partial f_s(p, r)}{\partial t} + F \frac{\partial f_s(p, r)}{\partial p} = \frac{\partial f_s(p, r) - \partial f_{0s}(p, r)}{\tau}, \quad \dots \dots \dots (3)$$

Where $F = \frac{dp}{dt} = eE$ is the constant electrostatic forces stand-in on the particles, and $f_s(p, r)$ is the Fermi distribution functions.

We utilize the method outlined in (Ohta *et al.*, 2006) to understand how the CNT transport properties depend on the energy E .

Equation 2.4 below, illustrates how the current density's longitudinal components are shaped $j=j_x$:

$$j(x) = \sigma(E)E + D(E) \frac{\nabla_x n}{n}. \quad \dots \dots \dots (4)$$

Expressions for $\sigma(E)$ and $D(E)$ of single-walled CNT for temperature distribution that is uniform. $T(r) = \text{constant}$ in a linear approach in $\nabla_x n$. The following formula describes $\sigma(E)$ of zigzag CNTs:

$$\sigma(E) = \sum_s \sum_m \int_{-\pi}^{\pi} dp_x A_{ms} m f_{0s}(p_x, x) \frac{E}{E^2 m^2 + 1} \times [\sin(mp_x) + Em \cos(mp_x)]. \quad \dots \dots (5)$$

The following form is the expression for $D(E)$ in CNTs of the "zig-zag" type:

$$D(E) = \sum_s \int_{-\pi}^{\pi} f_{0s}(p_x, x) \sum_m A_{ms} m \sum_{m'} A_{m's} m' \times \left\{ \frac{E^2(m^2 + m'^2) + 1}{K(E, m, m')} [EmR(E, m, m'p_x) + M(E, m, m'p_x)] + \frac{E^3(m'^2 - 2m^2 m') + Em'}{K(E, m, m')} \times T(E, m, m'p_x) \right\} dp_x + \sum_s \int_{-\pi}^{\pi} f_{0s}(p_x, x) \times \sum_m A_{ms} m \sum_{m'} A_{m's} m' \frac{F(E, m, m'p_x)}{P(E, m, m')} dp_x. \quad \dots \dots \dots (6)$$

Where the following notation is:

$$K(E, m, m') = [E^4(m^4 + m'^4 - 2m^2m'^2) + 2E^2(m^2 + m'^2) + 1][E^2m^2 + 1],$$

$$P(E, m, m') = (E^2m^2 + 1)^2(E^2m'^2 + 1),$$

$$R(E, m, m', p_x) = \cos(mp_x) \sin(m' p_x) + \cos(mp_x) \cos(m' p_x) - \sin(m p_x) \sin(m' p_x),$$

$$M(E, m, m', p_x) = \sin(mp_x) \sin(m' p_x) + \sin(mp_x) \cos(m' p_x) + \cos(m p_x) \sin(m' p_x),$$

$$T(E, m, m', p_x) = [\cos(mp_x) \cos(m' p_x) - Em \sin(mp_x) \cos(m' p_x)],$$

$$F(E, m, m', p_x) = [\sin(m' p_x) + Em \cos(m' p_x)] \times [\sin(m p_x) + 2Em \cos(m p_x) - E^2m^2 \sin(m p_x)],$$

A_{ms} And $A_{m's}$: are the Fourier expansion coefficients of the electron energy.

The order of expansion in the Fourier series is determined by the electron Fourier dispersion relationship in CNTs m and m' . The relative unit of measure electric field strength $E_0 = 4.7 \times 10^6 \text{ V/m}$ is used for the procedure of non-dimensionalization, the practicality of qualitative analysis and visualization.

Additionally, the effects of $E(x, t)$ directed along the ribbon's surface and applied along the x-axis on the temperature dependence of the bi-layer graphene nano-ribbons' transportation characteristics were investigated. The geometric configuration of a bi-layer graphene ribbon placed in an external constant electric field is shown in Fig. (2). The tape under discussion has hexagonal construction in bi-layers that are packed in an ABAB pattern. The system is taken into account by the Hubbard model (Georges, 1996), which uses the nearest neighbor approximation and only the energy of π -electron. Graphene layers are subjected to coulomb potentials U . The tight-binding approximation band structure allows for the expression of the dispersion equation for a bi-layer graphene tape in the type (Ohta *et al.*, 2006).

$$E_p^{\pm\pm}(U) = \pm \sqrt{\varepsilon_p^2 + \frac{\gamma^2}{2} + \frac{U^4}{4}} \pm \sqrt{\frac{\gamma^4}{4} + (\gamma^2 + U^2)\varepsilon_p^2}, \quad \dots \dots \dots (7)$$

Where the dispersion relation of single-layer graphene ε_p is determined by the formula (7)

$$\varepsilon_p = \pm t_0 \sqrt{1 + 4 \cos(ap_x) \cos\left(\frac{\pi s}{n}\right) + 4 \cos^2\left(\frac{\pi s}{n}\right)}, \quad \dots \dots \dots (8)$$

Table 1: Parameter Values for Equations

The Parameters	Values
b- The distance between nearby carbon atom in graphene	0.141 nm
$a=3b/2\hbar$	$\hbar$ is the Planck constant
t_0 - The integral of electrons hopping between nearby crystal lattice locations	$\approx 2.67\text{eV}$
γ -The hopping integral between layers	$\approx (0.4) \text{ eV}$
$p = (p_x, s)$	The graphene electron's quasi-momentum
p_x	Parallel to the sheet graphene quasi-momentum
s- The width of the graphene sheet is used to count the quantization's of the momentum components	1, 2, ..., n

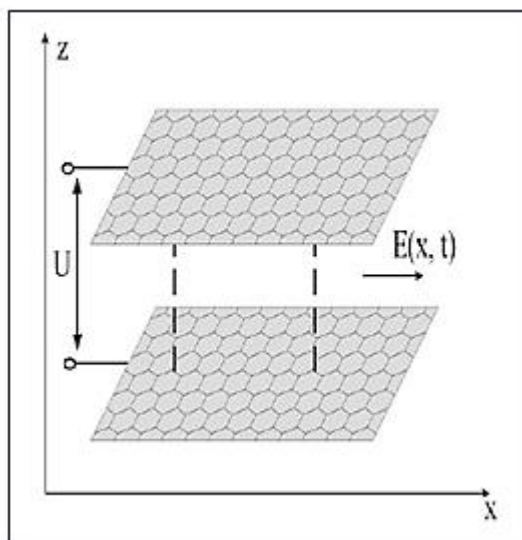


Fig. 2: Two-layer graphene ribbon in an external electric field. The field strength vector E is directed along the ribbon

The conduction and valence bands are denoted by various signs in the dispersion, respectively. Expressions for single-layer carbon nanotubes and bi-layer graphene tapes' specific $\sigma(E)$ and $D(E)$ are comparable. The acquired results of the temperature dependency of the transport properties for the types of carbon nanoparticles under consideration are shown graphically in the following section.

RESULTS AND DISCUSSION

Two different forms of nanostructures: Single-layer "zig-zag" carbon nanotubes and bi-layer graphene ribbons are used to illustrate how the transport properties of carbon derivatives depend on the temperature. The electron relaxation period is estimated to be 1.4×10^{-12} s (Dragoman, 2014). For the numerical analysis of the temperature dependences, semiconductor CNTs of the (10,0) type and bi-layer graphene tapes are considered. The relationship between the strength of E and $\sigma(E)$ of single-layer carbon nanotubes of the "zig-zag" type and bi-layer graphene tapes have property that is typical for semiconductor structures: as the external field's amplitude increases, it was first tends toward saturation before monotonically decreasing as the intensity increases, which is consistent with (Salimath *et al.*, 2014). This phenomenon can be explained by the fact that increasing the number of electrons is actually filling up all the potential states in the conduction band. It should also be noted that a periodic and restricted dispersion relations rule in semiconductor constructions typically exhibit a similar type of change in $\sigma(E)$ when they are subjected to an external electric field (Dykman, 1981). Fig. (3) shows the relationship between $\sigma(E)$ of semiconductor type (10.0) and the tension of the external constant electric field E at various temperatures including: $T = 10, 50, 100$ and 300 K (black, red, green and blue curves respectively). These four values of $\sigma(E)$ were obtained using formula (2.5).

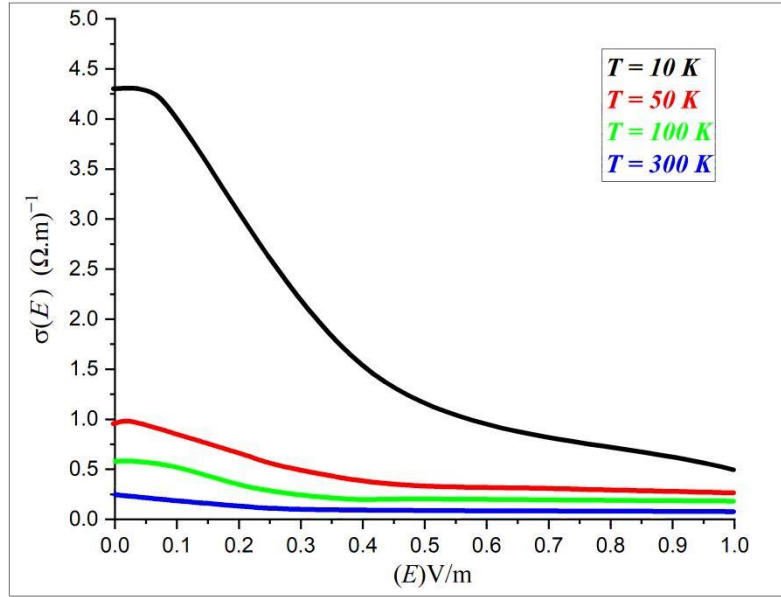


Fig. 3: Electrical conductivity $\sigma(E)$ of CNTs type (10,0) at various temperatures as a function of the strength of an external electric field E .

Fermi-Dirac distribution implies that as the temperature rises, the concentration of the free charge carriers should also rise in the conduction-band. Furthermore, increasing the temperature causes the conduction band to be filled up with low-energy quantum states, as a result of the degeneracy of the energy states has been doubled in the conduction band. On the other hand, $\sigma(E)$ coefficient decreases with rising the temperature because the fully filled states do not contribute to the substance's conductivity. The fact that the energy gap in the electronic spectrum is very small within the confines of the model under examination, which also ensures conducting qualities, should be taken into consideration. Regarding bi-layer carbon nanoribbons, as shown in Fig. (4), a similar type of dependency of $\sigma(E)$ on the magnitude of the strength of E is also found.

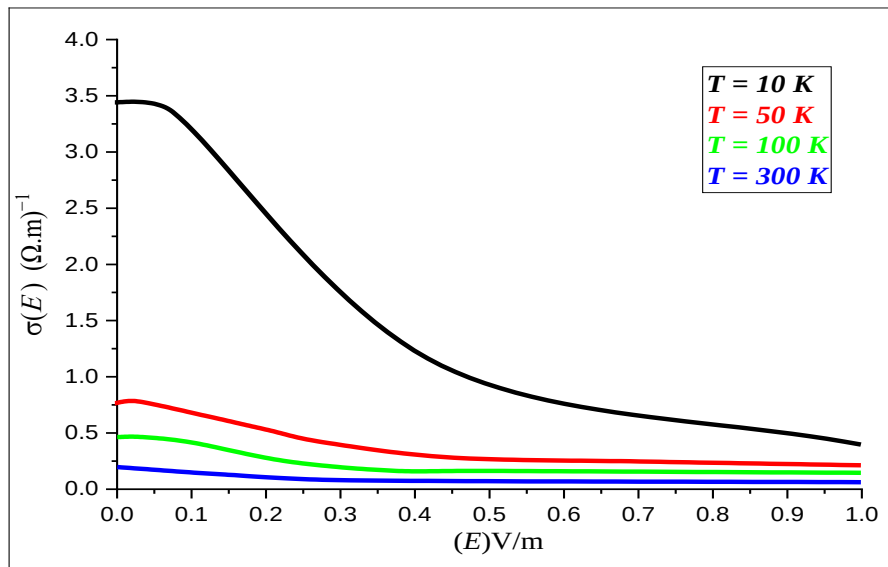


Fig. 4: Electrical conductivity $\sigma(E)$ of CNTs bi-layer type (10,0) at various temperatures as a function of the strength of an external electric field E .

As the temperature rises, the electrical conductivity coefficient decreases, which is explained by the reasons described above. It should be noted that the application of electrostatic potential and accounting for the jump of electro-nov between layers of tape has resulted in single-layer carbon nanotubes of the "zig-zag" type having a quantitatively higher $\sigma(E)$ than bi-layer carbon nanoribbons containing the same number of unit cells in the cross-section. A rise in the constant voltage across the layers of tape results in a reduction in $\sigma(E)$ (Buligin *et al.*, 1999). This behavior reflects by rearranging the Fermi level, which eventually raises the number of localized (degenerate) states in the electronic spectrum. For $D(E)$ calculations in Figs.(5 and 6) the applied transverse voltage between the graphene layers is 1 V. Figs.(5 and 6), also suggest that $D(E)$ of both single-layer "zig-zag" CNTs and bi-layer graphene tapes are temperature independent. These results of $D(E)$ calculations Figs. (5 and 6), were obtained by employing formula 2.6. This finding can be explained by the fact that, the concentration gradient is independent of the temperature and instead it characterized by the diffusion coefficient, which has a constant value.

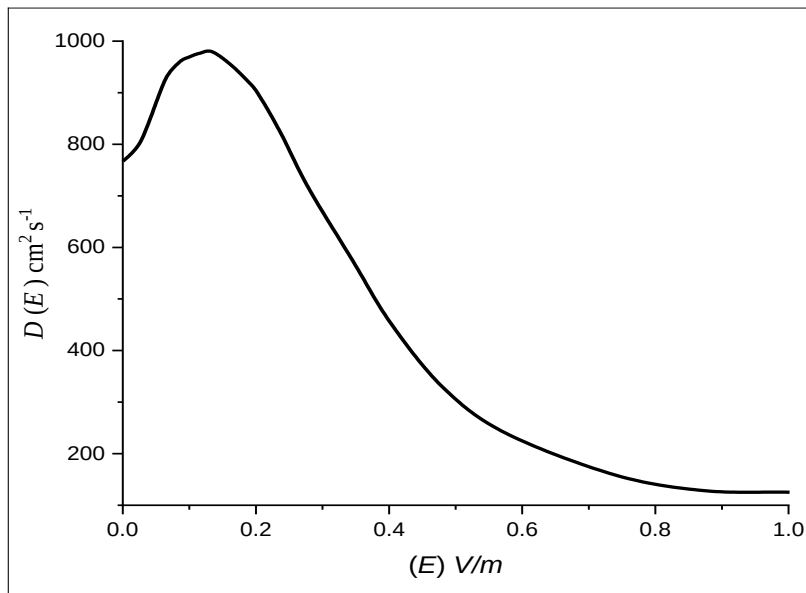


Fig. 5: $D(E)$ versus the strength of E , of CNTs type (10.0).

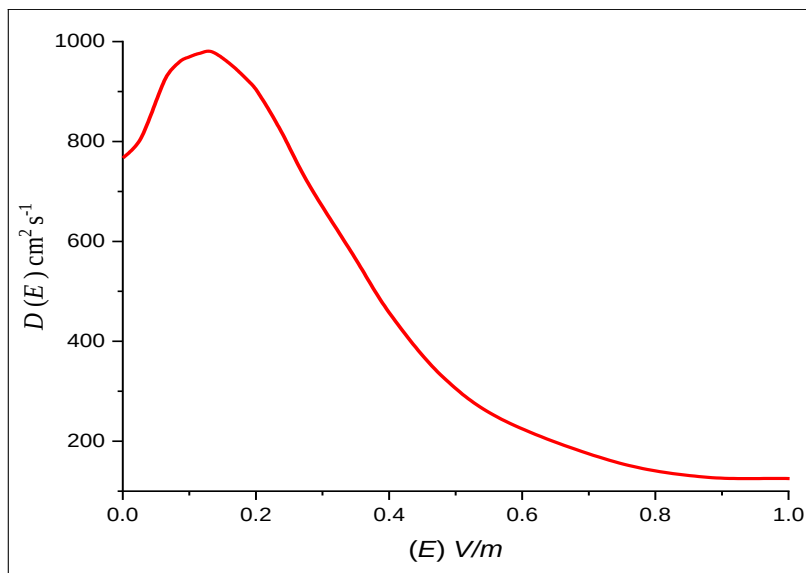


Fig. 6: The influence of the external electric field E , on $D(E)$ for bi-layer graphene tapes type (10.0)

In both single-layer and bi-layer carbon nanostructures, $D(E)$ relies nonlinearly on the strength of E . Initially increasing E causes the field to grow then decreases to a stationary value. Systems of periodic and constrained electron dispersion relations in general, exhibit the described transport phenomena in reference (Dykman, 1981). These key results can be applied to generate carbon nanoparticle-based composites and nano/ microelectronic components in addition to carbon nanoparticles with specified transport properties.

CONCLUSION

This research includes a theoretical analysis of the transport properties of carbon nanoparticle derivatives which involve quasi-one-dimensional (single-layer carbon nanotubes) and quasi-two-dimensional (bi-layer graphene nanoribbons). This study shows that for various temperatures including 10, 50, 100 and 300 K, the amplitude of the external constant electric field E has a nonlinear relationship with $\sigma(E)$ of carbon nanoparticles. It also explains how the $\sigma(E)$ coefficient decreases with increasing the temperature. On the other hand, both single-layer and bi-layer nanoparticle derivatives demonstrate a temperature-independent behavior of electron diffusion through the studied structures. This study also proves that $D(E)$ has a nonlinear dependence on the intensity of E for the explored structures.

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التحقيق النظري في الناقلية للأنابيب النانوية أحادية الجدار والجرافين ثنائي الطبقة

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الملخص

تمت دراسة خصائص النقل للعديد من مشتقات الجسيمات النانوية الكربونية، بما في ذلك الأنابيب النانوية أحادية الطبقة والجرافين ثنائي الطبقة، تحت مجال كهربائي ثابت خارجي. تم تحليل النتائج وتحديد كدالة للتقريب شبه الكلاسيكي لوقت الاسترخاء باستخدام معادلات بولتزمان الحركية. تم استخدام هذه الأساليب للحصول على العلاقات بين الموصلية الكهربائية σ (E) ومعامل انتشار الإلكترونات $D(E)$ في الهياكل النانوية الكربونية. تثبت هذه الدراسة أنه عندما ترتفع درجة الحرارة، تنخفض الموصلية الكهربائية σ (E) لكل من الهياكل النانوية الكربونية أحادية الطبقة وثنائية الطبقة. بالنسبة لمجموعة واسعة من درجات الحرارة، يعتمد سلوك التوصيل الكهربائي σ (E) للجسيمات النانوية المدروسة بشكل غير خطي على حجم المجال الكهربائي الخارجي (E). في المقابل، فإن معامل انتشار الإلكترون $D(E)$ مستقل عن درجة الحرارة لكل من الطبقات الفردية وثنائية. كما يوضح أن شدة المجال الكهربائي الخارجي لها تأثير غير خطي على معامل انتشار الإلكترون.

الكلمات الدالة: الأنابيب النانوية أحادية الجدار، الجرافين ثنائي الطبقة، التوصيل الكهربائي، انتشار الإلكترون، معادلات بولتزمان الحركية.