Pis'ma v ZhETF, vol. 97, iss. 7, pp. 465 – 468 © 2013 April 10

On the electronic spectrum in curved graphene nanoribbons

A. V. Zhukov[1)], R. Bouffanais, N. N. Konobeeva[+], M. B. Belonenko[*]

Singapore University of Technology and Design, 20 Dover Drive, 138682 Singapore

[+]*Volgograd State University, 400062 Volgograd, Russia*

[*]*Laboratory of Nanotechnology, Volgograd Institute of Business, 400048 Volgograd, Russia*

Submitted 22 February 2013

Using the formalism of the Dirac equation for curved space-time in the Friedmann model of a non-stationary universe, we calculate the electronic spectrum and density of states in curved graphene nanoribbons. Based on the obtained density of states we further study the current-voltage (IV) characteristics of the nanoribbon – metal tunnel junction. The dependence on the geometric characteristics of the nanoribbon has been revealed, showing a great influence of such parameters like the number of carbon atoms and the characteristic frequency of distortion.

DOI: 10.7868/S0370274X13070059

I. Introduction. Discovery of graphene and its unique characteristics [1, 2] allows to consider it as a basis for the electronics of the future. Nowadays the interest of researchers has increasingly shifted toward studying the properties of graphene, which can be modified in many different ways: impurities, defects, graphene nanoribbons, etc. [3, 4]. The latter is due to the fact that the pure graphene has no energy gap in its band structure and, consequently, the creation of various devices (e.g. analogs of transistors) is hardly feasible. The band structure of graphene in the Dirac points is degenerate, but any perturbation removes the degeneracy and results in the appearance of an energy gap in the spectrum. This particular specificity arises in graphene nanoribbons, which are restricted to one dimension. This leads to the quantization of the electron energy spectrum along a given direction, which therefore yields the appearance of an energy gap. Also, it is well known that the flat structure of graphene sheets is unstable [5, 6]; so that normally graphene has a wave-like curved surface. All these circumstances have stimulated recently the study of different modifications of a curved graphene [7, 8]. The long-wave approximation, which is widely used to describe the properties of electrons in graphene, leads to an analog of the Dirac equation, which in turn makes it easy to produce a generalization to the case when the graphene surface is curved [9]. Note that in this case the degeneracy in the Dirac points is removed and therefore it becomes possible to create various structures with different band gaps. Curvature of the graphene (see, e.g., [7]) leads also to a change in the electron density of states and, therefore, it is possible to change the whole set of electrical characteristics of the graphene sample. Apparently, the easiest way for an experimental verification of changes in the density of states is to study the tunneling current [10] through, e.g. a contact with the metal. All of the above form the impetus for the present study.

II. Electron spectrum. We consider the graphene nanoribbon in the Friedmann model of non-stationary universe [11]. Properties of electrons in the graphene nanoribbon in the long-wave approximation in the vicinity of the Dirac point will be described on the basis of the generalized Dirac equation for a curved space-time [9]:

$$\gamma^\mu(\partial_\mu - \Omega_\mu)\Psi = 0, \tag{1}$$

where ∂_μ is the partial derivative with respect to the coordinate μ, Ω_μ is the spin connection, and $\Psi = (\phi, \psi)^{\mathrm{T}}$ is the spinor, containing the wave functions describing the electrons in different sublattices of graphene near the Dirac point K. Dirac gamma-matrices γ^μ in a curved space-time are determined from the relation $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$, where $g^{\mu\nu}$ is the metric tensor.

As we know from the literature [9, 12], once the metric tensor $g_{\alpha\beta}$ is given, i.e.

$$\begin{gathered} ds^2 = g_{\alpha\beta}dx^\alpha dx^\beta, \\ g_{\alpha\beta}g^{\beta\gamma} = \delta^\gamma_\alpha, \end{gathered} \tag{2}$$

one can define the field of frames (tetrads)

$$\begin{gathered} g_{\alpha\beta} = e^a_\alpha e^b_\beta \eta_{ab}, \\ g^{\alpha\beta} = e^\alpha_a e^\beta_b \eta^{ab}, \\ \eta_{ab}\eta^{bc} = \delta^c_a, \end{gathered} \tag{3}$$

[1)]e-mail: alex_zhukov@sutd.edu.sg

where for the 2D curved surface $\eta_{ab} = \mathrm{diag}(1, -1, -1)$. Then

$$\Omega_\mu = \frac{1}{4}\gamma_a\gamma_b e^a_\lambda g^{\lambda\sigma}\left(\partial_\mu e^b_\sigma - \Gamma^\lambda_{\mu\sigma} e^b_\lambda\right), \tag{4}$$

where

$$\Gamma^\lambda_{\mu\sigma} = \frac{1}{2} g^{\lambda\nu}\left(g_{\sigma\nu,\mu} + g_{\nu\mu,\sigma} - g_{\mu\sigma,\nu}\right), \quad \gamma_\mu = e^\mu_a \gamma_a.$$

For a strained/curved graphene, constantly under the influence of an external variable mechanical force, the effect of this force leads to a periodic change in the distance between the atoms of graphene, which, in turn, leads to a change in the Fermi velocity, v_{F}. Using the analogy with a curved space-time, we can say that this force leads to a periodic change of spatial intervals, which, as is well known, is adequately described in the frame of the Friedmann non-stationary model. The metrics in the Friedmann non-stationary universe model has the form:

$$ds^2 = dt^2 - e^{f(t)}\left(dx^2 + dy^2\right), \tag{5}$$

where

$$e^{f(t)} = 1 + a\sin\omega_0 t.$$

Here a stands for the relative amplitude of the strain, while ω_0 is the characteristic frequency of oscillatory deformation. Then, the only following non-zero Christoffel symbols are

$$\Gamma^0_{11} = \Gamma^0_{22} = \frac{1}{2}e^{f(t)}f'(t); \quad \Gamma^1_{01} = \Gamma^2_{02} = \frac{f'(t)}{2},$$

so that

$$\Omega_0 = 0; \quad \Omega_1 = -\frac{1}{4}\gamma_0\gamma_1 f'(t)e^{f(t)/2};$$
$$\Omega_1 = -\frac{1}{4}\gamma_0\gamma_2 f'(t)e^{f(t)/2}.$$

Let us choose $\gamma_0 = \sigma_3$, $\gamma_1 = -i\sigma_2$, $\gamma_2 = -i\sigma_1$, where σ_i are the corresponding Pauli matrices. Then we obtain the following set of equations

$$\begin{aligned} &v_{\mathrm{F}}^{-1}\partial_t\phi + e^{-f(t)}\partial_{x_1}\psi + \frac{1}{4}f'(t)e^{-f(t)/2}\phi + \\ &\quad + ie^{-f(t)}\partial_{x_2}\psi - \frac{i}{4}f'(t)e^{-f(t)/2}\phi = 0, \\ &v_{\mathrm{F}}^{-1}\partial_t\psi - e^{-f(t)}\partial_{x_1}\phi - \frac{1}{4}f'(t)e^{-f(t)/2}\psi + \\ &\quad + ie^{-f(t)}\partial_{x_2}\phi - \frac{i}{4}f'(t)e^{-f(t)/2}\psi = 0, \end{aligned} \tag{6}$$

where we explicitly introduced the Fermi velocity for the flat graphene via $\partial_0 = v_{\mathrm{F}}^{-1}\partial_t$.

The solution of the system (6) can be found in the form

$$\begin{pmatrix}\phi\\ \psi\end{pmatrix} \to \begin{pmatrix}\phi\\ \psi\end{pmatrix}\exp\left(ip_x x + ip_y y\right),$$

yielding

$$\begin{aligned} &v_{\mathrm{F}}^{-1}\partial_t\phi + ip_x e^{-f(t)}\psi + \frac{1}{4}f'(t)e^{-f(t)/2}\phi - \\ &\quad - p_y e^{-f(t)}\psi - \frac{i}{4}f'(t)e^{-f(t)/2}\phi = 0, \\ &v_{\mathrm{F}}^{-1}\partial_t\psi - ip_x e^{-f(t)}\phi - \frac{1}{4}f'(t)e^{-f(t)/2}\psi - \\ &\quad - p_y e^{-f(t)}\phi - \frac{i}{4}f'(t)e^{-f(t)/2}\psi = 0. \end{aligned} \tag{7}$$

Let the function ϕ can be ansatz-sought through the equation

$$\phi_t + g\phi = 0,$$

where

$$g = \alpha v_{\mathrm{F}} f'(t)e^{-f(t)/2}, \quad \alpha = \frac{1-i}{4}.$$

Then the substitution $\phi \to \phi\exp\left(\int g dt\right)$, applied the set of Eq. (7) yields the non-linear Shrödinger equation with the excitation term (second one):

$$\phi_{tt} + \phi_t\left(f' + g^* - g\right) + |g|^2 e^{-2f}\phi = 0. \tag{8}$$

Let us choose the trial unexcited function in the form $\phi(t) = \phi_0 e^{i\omega t}$. In the non-perturbed case ($f = 0$), we obtain the spectrum

$$\omega^2 = |\mathbf{p}|^2.$$

The wave vector p is found from the boundary conditions at the ends of the nanoribbon. In our particular case we have chosen the armchair-type ribbon [8, 13], hence

$$p_n = \frac{2\pi}{3a_0}\left(\frac{2M + 1 + n}{2M + 1}\right), \tag{9}$$

where a_0 is the interatomic distance in the carbon lattice, M is the number of atoms along the nanoribbon axis, and n is the quantum number.

Let us calculate the first energy correction $V = \int \psi^\dagger \hat{V}\psi dx$ with $\psi = A\sin(p_n x_1)$ and $\hat{V} = (f' + g^* - g)\partial_t$. The integration is done over the interval $[0, (3M+1)\,a_0]$, and results in

$$V = \frac{p_n}{2L}\frac{a\omega_0\cos\omega_0 t}{1 + a\sin\omega_0 t}\left(1 + \frac{1}{\sqrt{1 + a\sin\omega_0 t}}\right)\sin(2p_n t). \tag{10}$$

The dependence of the energy correction on the atom numbers M is demonstrated in Fig. 1. This dependence

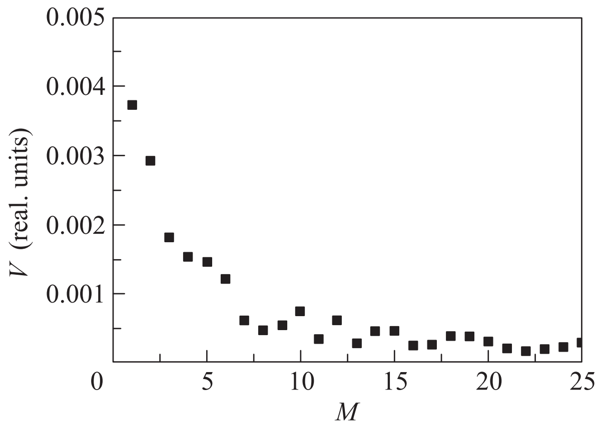

Fig. 1. Dependence of the energy correction V, caused by the perturbation $\hat{V}$, on the number of atoms M along the axis of the nanoribbon ($n = 1$)

has a step-like form, which is associated with the quantization of the electron spectrum in graphene nanoribbons according to Eq. (9). Note that this is similar to the dependence of the energy gap in zigzag-type carbon nanotubes [14], which also arises from the quantization of the electron spectrum in the direction along the circumference of the nanotube.

Furthermore, it is worth characterizing the dependence of V on the parameters ω_0 and n. This dependence is shown in Fig. and demonstrates that with the

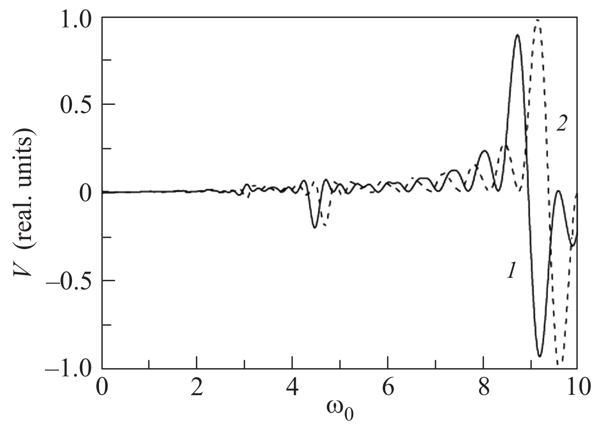

Fig. 2. Dependence of the energy correction V, caused by the perturbation $\hat{V}$, on the parameter ω_0 for $M = 20$, $n = 1$ (*1*) and $n = 3$ (*2*)

increase of the characteristic frequency ω_0, we observe a periodic change of the correction to the energy of the electrons. With increasing quantum number n, we observe a shift to the right and a remarkable increase in the amplitude.

III. Tunnel characteristics. Within the framework of the Kubo response theory [15], the current is given by

$$J = 4\pi e|T|^2 \int_{-\infty}^{\infty} d\mathcal{E}\nu^{(A)}(\mathcal{E} + eV)\nu^{(B)}(\mathcal{E}) \times \times \{n_f(\mathcal{E}) - n_f(\mathcal{E} + eV)\}, \tag{11}$$

where $n_f(\mathcal{E})$ is the equilibrium distribution of fermions with the energy $\mathcal{E}$. Here the tunnel densities of states $\nu^{(A,B)}$ are given by

$$\nu^{(A)}(\mathcal{E}) = \sum_p \delta\left(\mathcal{E} - \mathcal{E}_p^{(A)}\right), \ \nu^{(B)}(\mathcal{E}) = \sum_q \delta\left(\mathcal{E} - \mathcal{E}_q^{(B)}\right).$$

Let us take the electronic spectrum for the graphene nanoribbon given by Eq. (8) while accounting for the correction term given by Eq. (10). Note, we consider that the electron in a metal with a contact is supposed to have the free-like spectrum

$$\mathcal{E}_p^{(A)} = \frac{p^2}{2m}. \tag{12}$$

After computing the integrals in Eq. (11), we obtain the current-voltage characteristics of the contact shown in Fig. 3. It shows the asymmetric behavior of current ver-

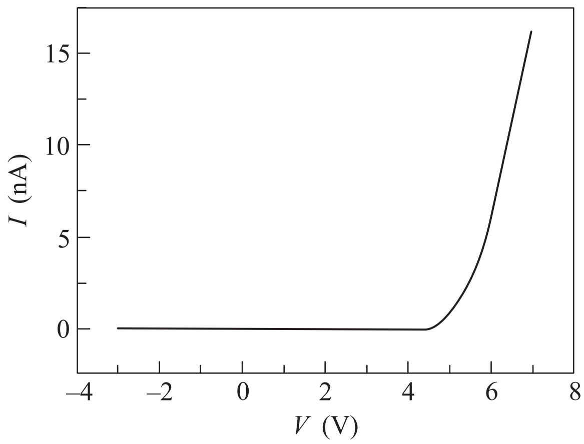

Fig. 3. IV-characteristics of a curved nanoribbon-metal tunnel junction

sus voltage applied to the contact. This is due to both, the peculiarities of the electronic structure (density of states) of the metal and graphene nanoribbon, and the processes of carrier recombination in the transition contact, which dominates over the thermal processes when $V > 0$. Similar behavior is observed for germanium, and especially for silicon diodes. Note that this dependence can have important practical applications in the study of nanocontacts and the design of diodes based on graphene nanoribbons.

IV. Conclusions. In conclusion, we formulate the main outcomes of the work done.

i) We have derived the effective equation describing the electrons in a curved graphene nanoribbon for the tunneling current through the nanoribbon-metal contact within the frame of the non-stationary Friedmann model.

ii) The dependence of the electronic spectrum of the nanoribbon on the space curvature is revealed. In general, the first correction to the spectrum is determined by the number of atoms along the axis of the nanoribbon M, as well as by the characteristic deformation frequency ω_0.

iii) We derive the IV-characteristics for a graphene nanoribbon-metal contact, which is similar to the well-known characteristics of classical diodes.

A.V. Zhukov and R. Bouffanais are financially supported by the SUTD-MIT International Design Centre (IDC). M.B. Belonenko and N.N. Konobeeva acknowledge a support from the Russian Foundation for Fundamental Research.

1. K. S. Novoselov, A. K. Geim, S. V. Morozov et al., Science **306**, 666 (2004).
2. K. S. Novoselov, A. K. Geim, S. V. Morozov et al., Nature **438**, 197 (2005).
3. Y. Zhang, J. W. Tan, H. L. Stormer, and P. Kim, Nature **438**, 201 (2005).
4. S. Stankovich, D. A. Dikin, G. H. Dommett et al., Nature **442**, 282 (2006).
5. A. Cortijo and M. A. H. Vozmediano, Nucl. Phys. B **763**, 293 (2007).
6. A. Cortijo and M. A. H. Vozmediano, Europhys. Lett. **77**, 47002 (2007).
7. D. V. Kolesnikov and V. A. Osipov, JETP Lett. **87**, 419 (2008).
8. L. Brey and H. A. Fertig, Phys. Rev. B **73**, 235411 (2006).
9. M. A. H. Vozmediano, M. I. Katsnelson, and F. Guinea, Phys. Rep. **296**, 109 (2010).
10. M. B. Belonenko, N. G. Lebedev, and N. N. Yanyushkina, J. of Nanophotonics **4**, 041670 (2010).
11. L. D. Landau and E. M. Lifshitz, *The Classical Theory of Fields*, 4th Ed., Butterworth-Heinemann, 2000.
12. N. D. Birrell and P. C. W. Davies, *Quantum Fields in Curved Space*, Cambridge University Press, 1984.
13. M. B. Belonenko, N. G. Lebedev, N. N. Yanyushkina et al., Sol. State Comm. **151**, 1147 (2011).
14. M. S. Dresselhaus, G. Dresselhaus, and P. Avouris, *Carbon Nanotubes: Synthesis, Structure, Properties, and Applications*, Springer, 2001.
15. R. Kubo, J. Phys. Soc. Jap. **12**, 570 (1957).