

Tunneling of the Dirac Quasiparticles Through the Fermi Velocity Barriers Based on the Gapped Graphene



A. M. Korol, N. V. Medvid, A. I. Sokolenko, and O. Shevchenko

Abstract The transmission of ultrarelativistic quasi-electrons through barrier structures based on the gapped graphene is studied. The transmission coefficient is calculated within the continuum model using the solution of the Dirac-type equation for two types of structures in which the barriers are created due to the fact that the Fermi velocity acquires different values in the barrier and out-of-barrier regions. In one structure, the barrier has a step-like shape, the other is a single barrier resonance tunneling structure. The results of a detailed analysis of the transmission spectra depending on the parameters of the problem: the energy of the quasiparticles, the angle of their incidence on the barrier, the size of the energy gap, and the thickness of the barrier, are presented.

Keywords Gapped graphene · Transmission coefficient · Velocity barriers

1 Introduction

As known [1], graphene has a number of unique properties, which is why a large number of works are devoted to its study. Among these properties, we will name only some: a linear dispersion relation for the quasiparticles, unusual quantum Hall effect, the property of chirality, the Klein tunneling, high mobility, ballistic transport, etc. In addition, the use of graphene promises to be very promising in modern nanoelectronics. Charge carriers in graphene are fermions with a pseudospin equal to 0.5, and they obey an equation similar to Dirac relativistic equation. The key parameter that characterizes the dispersion relation of the Dirac quasiparticles is the Fermi velocity. Therefore, it is clear that significant efforts have been made to be able to control this value and also to use this control in practice [2–13]. For this purpose, a number of

A. M. Korol (✉) · N. V. Medvid · A. I. Sokolenko · O. Shevchenko
National University for Food Technologies, Volodymyrska Str., 68, Kyiv, Ukraine
e-mail: korolam@ukr.net

A. M. Korol
Laboratory On Quantum Theory in Linköping, International Society for Independent Research (ISIR), Box 8017, 58080 Linköping, Sweden

© The Author(s), under exclusive license to Springer Nature Switzerland AG 2023
O. Fesenko and L. Yatsenko (eds.), *Nanomaterials and Nanocomposites, Nanostructure Surfaces, and Their Applications*, Springer Proceedings in Physics 279,
https://doi.org/10.1007/978-3-031-18096-5_14

different methods were proposed and experimentally tested. Many articles have been published examining the effect of Fermi velocity on the characteristics of various graphene structures. The Fermi velocity can take different values in different parts of the given structures, i.e., be a spatially dependent quantity. In particular, in [2–12], the influence of the Fermi velocity on such structures as one- and two-barrier resonance-tunneling structures, as well as on different superlattices was analyzed. Both electrostatic and magnetic barriers were taken into account. Despite the good prospects for the use of graphene in practice, it has some drawbacks. From the point of view of the use of graphene as an element of transistor circuits, one of such defects is the Klein paradox, according to which graphene has a high transmission coefficient T for carriers the angle of incidence of which on the barrier θ is normal or close to normal (and $T = 1$ for $\theta = 0$). To correct this defect, various approaches have been proposed, one of which is the use of graphene with an energy gap (the gapped graphene). Motivated by the above, in this paper, we analyze the tunneling process in structures, part of which is the gapped graphene and show in which cases the effect of the energy gap on the transmission coefficient is significant. We must note here that the obtained expression for the transmission rates accounts for the π phase change of the transmitted wave function. It is known that taking into account this change leads to significant changes in the transmission spectra [14, 15], in particular, it manifests the phenomenon of the supertunneling [13]. We analyze the tunneling process in two structures: one with the step-like Fermi velocity barrier and another containing the single barrier with a finite width. The barrier region of these structures consists of the gapped graphene.

2 Model and Formulae

Assume that there is the single rectangular one-dimensional Fermi velocity barrier with the width d , the interfaces coordinates being $x_l = 0$ and $x_r = d$ for the left and the right interfaces, respectively. This barrier (of a rectangular shape) is created due to the fact that the Fermi velocity has different values in the barrier and out-of-barrier regions of the given structure; that is, we believe that both out-of-barrier regions consist of the massless graphene, and the barrier area is represented by the gapped graphene. The low-energy fermion excitations in the considered structure based on the gapped graphene can be described by the following Hamiltonian (see, e.g., [1]):

$$H = -iv_F \left(\sigma_x \frac{\partial}{\partial x} + \sigma_y \frac{\partial}{\partial y} \right) + \Delta \sigma_z \quad (1)$$

where Δ is half of the width of the energy gap, $\Delta = mv_F^2$, m quasielectron mass, v_F the Fermi velocity, σ_x and σ_y are the Pauli matrices, and σ_0 the unit matrix, and we put $\hbar = 1$.

In the case when the Fermi velocity varies in space, this Hamiltonian is not the hermitian one [16, 17]. Assume that the Fermi velocity depends on the coordinate x (only). As usual in the relevant cases, it is assumed also that the barrier width is much larger than the near-interface regions associated with the gradual change in the Fermi velocity. Then in accordance with the considerations made in [16, 17], we may present the Hamiltonian of the problem as follows:

$$H = -i\sqrt{v_F(x)}\left[\sigma_x \frac{\partial}{\partial x} \sqrt{v_F(x)} + \sqrt{v_F(x)}\sigma_y \frac{\partial}{\partial y}\right] + \Delta\sigma_z \quad (2)$$

and now it has the hermitian form [16, 17]. We must keep in mind that the derivative acts on the product $\sqrt{v_F(x)}\psi = \phi$ where ψ are the spinorial eigenfunctions. If the electron wave moves along the axis Ox from the left to the right, then for the wave functions in the left and in the right out-of-barrier regions it is possible to write, respectively [13, 15]:

$$\begin{aligned} \psi_l(x, y) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i(\pi - \theta)} \end{pmatrix} e^{i(-k_x x + k_y y)} \\ \psi_r(x, y) &= \frac{t}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix} e^{i(k_x x + k_y y)} \end{aligned}$$

for the barrier region

$$\begin{aligned} \psi_b(x, y) &= \frac{a}{\sqrt{2}} \begin{pmatrix} \gamma \\ \delta e^{i(\varphi + \pi)} \end{pmatrix} e^{i(q_x x + k_y y)} + \frac{b}{\sqrt{2}} \begin{pmatrix} \gamma \\ \delta e^{-i\varphi} \end{pmatrix} e^{-i(q_x x + k_y y)} \\ \gamma &= \sqrt{1 + \Delta / \sqrt{\Delta^2 + v_{F2}^2 q_x^2}}, \\ \delta &= \sqrt{1 - \Delta / \sqrt{\Delta^2 + v_{F2}^2 q_x^2}} \\ k_x &= \frac{E \cos \theta}{v_{F1}}, \quad q_x = \sqrt{\frac{E^2 - \Delta^2}{v_{F2}^2} - k_y^2}, \quad \theta = \arctan\left(\frac{k_y}{k_x}\right), \end{aligned} \quad (3)$$

and we assume that energy $E > 0$.

Using the following boundary conditions ([16, 17])

$$\begin{aligned} \sqrt{v_{F1}}\psi_l(x = 0^-) &= \sqrt{v_{F2}}\psi_b(x = 0^+) \\ \sqrt{v_{F2}}\psi_b(x = d^-) &= \sqrt{v_{F1}}\psi_r(x = d^+) \end{aligned} \quad (4)$$

one can find the coefficient t in expressions for the wave functions, and hence, the transmission coefficient $T = |t|^2$:

$$T(E, \varphi) = \rho \cos^2 \theta \cos^2 \varphi^2 / \left\{ \rho \cos^2 \theta \cos^2 \varphi^2 \cos(q_x d)^2 + \sin(q_x d)^2 [1 - \rho \sin(\theta) \sin(\varphi)]^2 \right\},$$

$$\rho = \frac{\varepsilon K}{\sqrt{\Delta^2 + (\varepsilon K)^2}}, K = \sqrt{k_x^2 + k_y^2}, \varepsilon = v_{F2} / v_{F1}, \tag{5}$$

v_{F2}, v_{F1} , being the Fermi velocity in the barrier and in the out-of-barrier regions, respectively. Using a similar approach, we can also derive the expression for the transfer coefficient T for a structure with a step-like barrier. The difference is that this structure consists of only two parts, the right of which is a semi-infinite Fermi velocity barrier and the left one is the pristine graphene. As in the above case of the single barrier with a finite width, the dispersion relation is expressed by formulas (3) in the out-of-barrier and in the barrier regions, respectively.

3 Results and Discussions

Figure 1 shows the dependence of the transmission coefficient T on an angle of incidence of quasielectrons on the barrier in a step-like structure. The Fermi velocity in the right part of the structure differs from the velocity in the left part so that the right part is a barrier for quasielectrons.

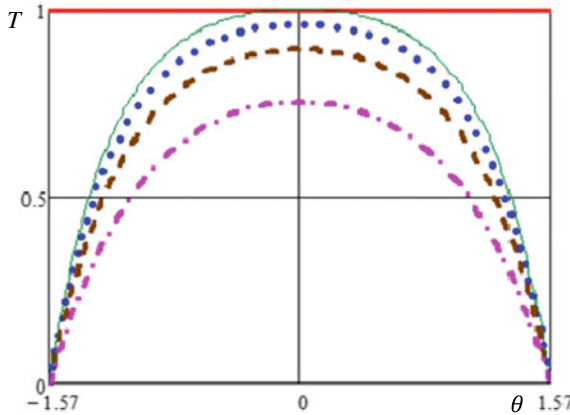


Fig. 1 Dependence of the transmission coefficient T on the incidence angle θ for the step-like structure. The values of the parameters for Fig. 1 are as follows: $E = 0.5, d = 1, \varepsilon = 0.3$ for all curves except for thick solid (red online) one for which $\varepsilon = 1; \Delta = 0$ for thick and thin solid (green) lines and $\Delta = 0.2, 0.3, 0.4$ for the dotted (blue), dashed (brown), and dashed-dotted (magenta) lines, respectively; the quantity θ is given in radians for all figures

Characterizing the presented in Fig. 1 dependence, we note the following: 1. Graph $T(E)$ has a pronounced angular dependence, and the barrier is the most transparent for the normal incidence of particles ($\theta = 0$) and its vicinity. 2. There is a marked decrease in T for all angles of incidence and its value increases with increasing energy gap Δ . 3. The Klein paradox disappears, i.e., the transmission for a normal incidence is not perfect. 4. The values of T significantly depend on the parameter ε . Note also that for many parameter values, the formation of the dependence $T(E)$ is influenced by the so-called critical angle. It is understood as such an angle that for all incidence angles greater than the critical one transmission rates falls sharply. The value of the critical angle can be derived using the Snell law and it is equal to

$$\theta_c = \arcsin\left(\sqrt{(E^2 - \Delta^2)} / E\varepsilon\right) \tag{6}$$

A horizontal solid (red) line, the value of T is the maximum ($T = 1$) for any angle of incidence. It refers to values: $\Delta = 0, \varepsilon = 1$, that is, to absence of the barrier.

It is seen that this dependence is not monotonic; its important feature is the presence of a maximum for a certain value of ε . Before reaching this maximum value of ε , the function $T(E)$ increases quite smoothly, and then falls sharply. At rather big values of Δ , the specified maximum does not take place any more. But note that such Δ values are already close to those that can be obtained in practice.

Regarding the dependence of T on energy of incident quasielectrons E , it should be noted that this dependence for the step-like barrier is monotonic, namely the value of T increases with increasing E . (Naturally, exceptions are small values of energy which are comparable to Δ). Obviously, the growth rate depends on the values of all parameters of the problem.

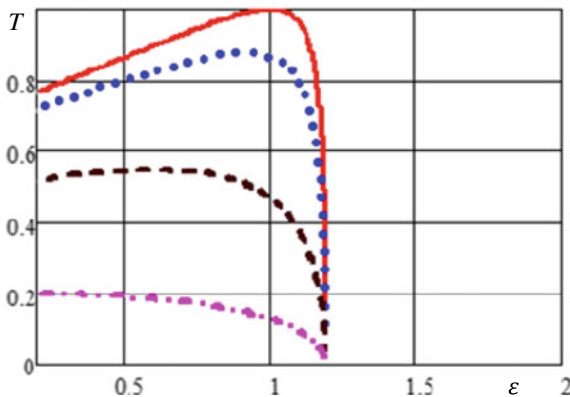


Fig. 2 Dependence of the transmission coefficient T on the parameter ε for the step-like structure. The values of the parameters for Fig. 2 are as follows: $E = 0.5, d = 1, \theta = 1$ for all curves, $\Delta = 0, 0.2, 0.4, 0.49$ for the solid (red), dotted (blue), dashed (brown), and dashed-dotted (magenta) lines, respectively

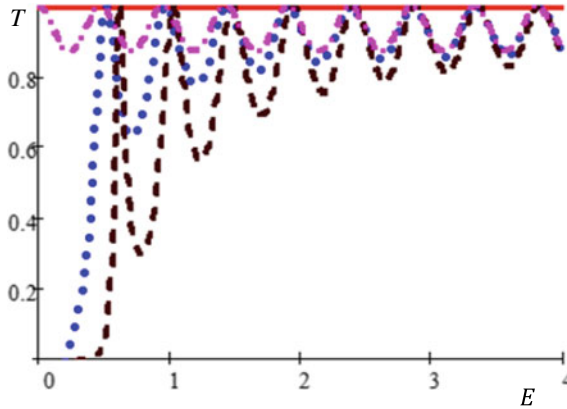


Fig. 3 Dependence of the transmission coefficient T on the quasiparticle energy E for the single barrier structure. The values of the parameters are as follows: $\theta = 0.5$, $d = 2$ for all lines; $\Delta = 0$, $\varepsilon = 1$ for the solid (red) line; $\Delta = 0$, $\varepsilon = 0.3$ for the dashed-dotted (magenta) curve; $\varepsilon = 0.3$, $\Delta = 0.2$, 0.4 for the dotted (blue) and dashed (brown) curves, respectively

The dependence of T on Δ for a given structure is also monotonic: The value of T decreases with increasing Δ ; here, it should be borne in mind that there may be different slopes of function $T(\Delta)$ for different delta values depending on the values of the problem parameters.

Figure 3 shows the dependence of T on the quasiparticles energy E for a structure with a single barrier of finite thickness d . This dependence is radically different from the similar one for a step-shaped barrier. Here, it is primarily characterized by the presence of numerous peaks with a maximum value of $T = 1$. These maxima are related to the presence in the expression for the transmission coefficient of the term $\sin(qd)$, which is zeroed under the condition $qd = n\pi$, as a result of which T becomes equal to 1. Thus, these maxima are Fabry–Perot-type resonances.

Their position on the energy axis is determined by the following formula.

$$d\sqrt{\frac{E^2 - \Delta^2}{\varepsilon^2} - k_y^2} = n\pi, \quad (7)$$

where $n = 1, 2, 3 \dots$

It follows from this formula that a smaller value of ε corresponds to a larger number of oscillations in a given range of Δ values. According to it, increasing the thickness of the barrier d facilitates the formation of Fabry–Perot resonances.

In particular, it follows from this formula that the energy position of the Fabry–Perot resonance data depends on the magnitude of Δ , which is confirmed by Fig. 3. The horizontal line with the value of $T = 1$ in Fig. 3 corresponds to the case of massless graphene and the value of $\varepsilon = 1$, i.e., the actual absence of the Fermi velocity barrier. If the barrier is present ($\varepsilon \neq 0$) but $\Delta = 0$, the dependence

$T(E)$ is an oscillating curve with the same amplitude of oscillations along the energy axis.

The fact that the presence of even a very small energy gap leads to noticeable changes in the spectrum of $T(E)$ is noteworthy (compare the dotted and dashed curves with the dashed-dotted one). It is seen in Fig. 3 that there is a wide transmission gap in the spectrum for small energy values. Its origin is due to the fact that the electron wave becomes evanescent at energies close to zero. The transmission gap width is very sensitive to changes in ε , and it increases rapidly with increasing ε (see Fig. 4). Also the transmission gap widens with increasing of the energy gap Δ or of the barrier thickness d . The number of Fabry–Perot-type resonances increases sharply with increasing in ε as well as in the barrier thickness. It is also seen that the difference in the effect of the Δ on T depends significantly on the value of ε . At the same time, the maxima associated with Fabry–Perot resonances remain equal to one; their position on the energy axis changes and the displacement increases with increasing Δ (according to formula (7)).

The plot of the $T(E)$ dependence for big values of beta is given by Fig. 4. We see that the oscillation period is much larger in comparison with that of Fig. 3.

Figure 5 provides the $T(\theta)$ dependence for the single barrier structure. The solid line refers to the case of $\varepsilon = 1, \Delta = 0$. Comparing Figs. 1 and 5 (which have the same values of the parameters), it is obvious that the effect of delta on T is much stronger for the single barrier structure than for the step-like one.

Figure 6 elucidates the T vs Δ dependence. One of the main conclusions that can be made on the basis of the dependence $T(\Delta)$ in Fig. 6 is that the transmission coefficient significantly depends on the size of the energy gap, namely that the presence of the gap can lead to a significant reduction of T and the decrease in T with increasing Δ may be quite sharp. The monotonic decreasing of T with increasing Δ takes place at the value of $\varepsilon > 1$ (for most values of the problem parameters).

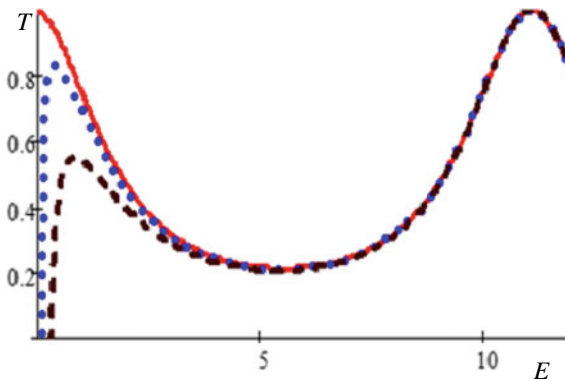


Fig. 4 Dependence of the transmission coefficient T on the quasiparticle energy E for the single barrier structure. The values of the parameters are as follows: $\theta = 0.5, d = 2, \varepsilon = 2$ for all lines; $\Delta = 0$ for the solid (red) line; $\Delta = 0.2, 0.4$ for the dotted (blue) and dashed (brown) curves, respectively

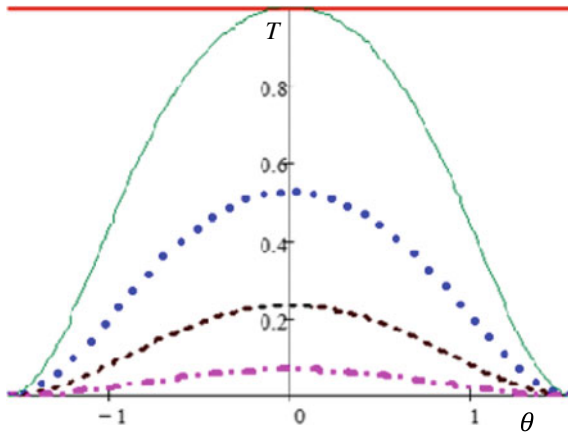


Fig. 5 Dependence of the transmission coefficient T on the incidence angle θ for the single barrier structure. The values of the parameters for Fig. 5 are as follows: $E = 0.5$, $d = 1$, $\varepsilon = 0.3$ for all curves except for thick solid (red online) one for which $\varepsilon = 1$; $\Delta = 0$ for thick and thin solid (green) lines and $\Delta = 0.2, 0.3, 0.4$ for the dotted (blue), dashed (brown), and dashed-dotted (magenta) lines, respectively

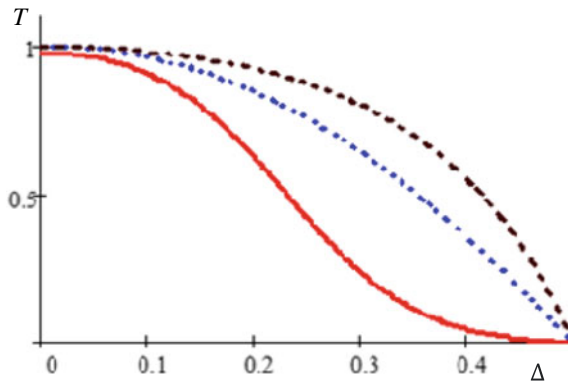


Fig. 6 Dependence of the transmission coefficient T on the energy Δ for the single barrier structure. The values of the parameters are as follows: $E = 0.5$, $\theta = 0.3$, $d = 1$ for all lines; $\varepsilon = 0.2, 1, 1.5$ for the dotted (blue) and dashed (brown) curves, respectively

It is also important that the dependence of $T(\Delta)$ can be oscillating one. This possibility follows from the formula for T (5) and is confirmed by Fig. 7. The maximum value of $T(\Delta) = 1$ corresponds to the resonances of the Fabry–Perot type. It follows from this formula that a smaller value of ε corresponds to a larger number of oscillations in a given range of Δ values.

In case of a normal incidence of massless particles on the barrier, the Klein tunneling is observed, for which $T = 1$ in the entire energy range. It is known that it also occurs in the presence of velocity barriers ($T = 1, \theta = 0, \varepsilon \neq 1$) [2–12].

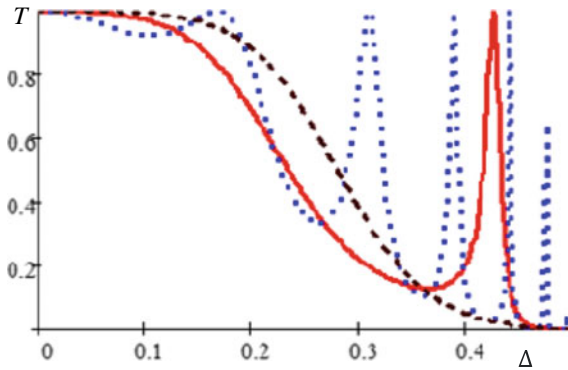


Fig. 7 Dependence of the transmission coefficient T on the energy gap Δ for the single barrier structure. The values of the parameters are as follows: $E = 0.5, \theta = 0, d = 12$ for all lines; $\varepsilon = 0.3, 1, 2$ for the dotted (blue), dashed (brown), and solid (red) curves, respectively

In case of massive particles ($\Delta \neq 0$), the Klein tunneling is suppressed, and the value of T decreases with increasing Δ .

Figure 8 represents the dependence of $T(\varepsilon)$. It has a pronounced oscillating character for small values of ε ($\varepsilon < 1$ for most values of other parameters), and the “period” of oscillations increases with increasing ε . The maximum values of T are equal to one and correspond to the Fabry–Perot-type resonances. The values of T decrease sharply in the intervals of energies between the peaks. There is also a significant difference in the magnitude of T for different Δ values.

Figure 9 illustrates the dependence of T on the barrier thickness d for different Δ and ε values. The horizontal line with $T = 1$ refers to the case: $\Delta = 0, \varepsilon = 1$. For nonzero Δ values, it is possible to observe two types of the function $T(d)$. For small values of ε , this function is an oscillating curve, and for sufficiently large values of ε ,

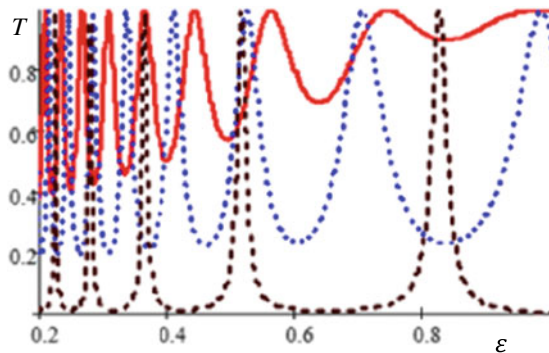


Fig. 8 Dependence of the transmission coefficient T on ε for the single barrier structure. The values of the parameters are as follows: $E = 0.5, \theta = 1, d = 12$ for all lines; $\Delta = 0, 0.2, 0.4$ for the solid (red), dotted (blue), and dashed (brown) curves, respectively

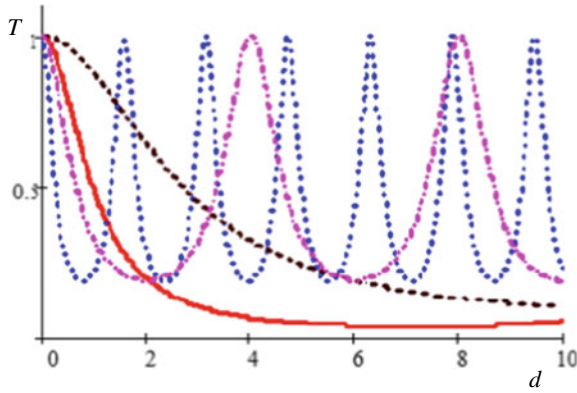


Fig. 9 Dependence of the transmission coefficient T on the barrier thickness d for different Δ and ε values for the single barrier structure. The values of the parameters are as follows: $E = 0.5$, $\theta = 0.4$, $\Delta = 0.3$, for all lines; $\varepsilon = 1, 0.2, 0.5, 2$ for the solid (red), dotted (blue), dashed-dotted (magenta), and dashed (brown) curves, respectively

the function $T(d)$ is represented by a descending curve—as in the case of conventional tunneling (see the dashed-dotted, dotted and the dashed, and solid lines, respectively, in Fig. 9). More massive particles give values of T significantly smaller than less massive ones. The number of oscillations in a given range of barrier thicknesses is noticeably smaller for more massive particles (compare the dashed-dotted and the dotted curves).

4 Conclusions

The two graphene-based structures are explored in this text: one with the step-like Fermi velocity barrier and another containing the single Fermi velocity barrier of a finite width. All out-of-barrier regions consist of the massless graphene, and the barrier area is represented by the gapped graphene. Some features of the transmission spectra (dependences of the transmission rates T on the parameter values) are common for both considered structures, namely: 1) magnitude of T is rapidly reduced with increasing in the energy gap (Δ) value (or the quasiparticle mass m); 2) spectra are highly anisotropic; that is, values of T markedly depend on the angle of incidence of the quasiparticle on the barrier θ ; 3) function $T(\theta)$ oscillates with the parameter values, in particular with the $\varepsilon = v_{F2}/v_{F1}$ value; and 4) the Klein tunneling is suppressed for the case of $m \neq 0$ ($\Delta \neq 0$). For the step-like barrier, the function $T(E)$ (E quasiparticle energy) is the monotonic and increasing with E one; there are no resonant energies. The function $T(\varepsilon)$ can reveal the pronounced maximum, and this function drops sharply to zero after reaching the maximum. For the rectangular barrier structure with a finite barrier width, a lot of maxima can be observed

in the $T(E)$ dependence as well as in the $T(\varepsilon)$ function—these are the Fabry–Perot-type resonances. The spectra $T(d)$ (d being the barrier width) is characterized by the following features. For nonzero Δ values, it is possible to observe two types of the function $T(d)$. For small values of ε , this function is an oscillating curve, and for sufficiently large values of ε , the function $T(d)$ is represented by a descending curve—as in the case of the conventional tunneling. More massive particles give values of T significantly smaller than less massive ones. The results of this work can be used in graphene-based nanoelectronics.

References

1. Neto AHC, Guinea F, Peres NMR, Novoselov KS, Geim AK (2009) The electronic properties of graphene. *Rev Mod Phys* 81:109
2. Liu L, Li Y-X, Liu J (2012) Transport properties of Dirac electrons in graphene based double velocity-barrier structures in electric and magnetic fields. *Phys Letters A* 376:3342–3350
3. Wang Y, Liu Y, Wang B (2013) Resonant tunneling and enhanced goos-hänchen shift in graphene double velocity barrier structure. *Phys E* 53:186–192
4. Sun L, Fang C, Liang T (2013) Novel transport properties in monolayer graphene with velocity modulation. *Chin Phys Lett* 30:047201
5. Raoux A, Polini M, Asgari R, Hamilton AR, Fasio R, Macdonald AH (2010) Velocity-modulation control of electron-wave propagation in graphene. *Phys Rev B* 81:073407
6. Concha A, Tešanović Z (2010) Effect of a velocity barrier on the ballistic transport of Dirac fermions. *Phys Rev B* 82:033413
7. Yuan JH, Zhang JJ, Zeng QJ, Zhang JP, Cheng Z (2011) Tunneling of Dirac fermions in graphene through a velocity barrier with modulated by magnetic fields. *Phys B* 406:4214–4220
8. Krstajic PM, Vasilopoulos P (2011) Ballistic transport through graphene nanostructures of velocity and potential barriers. *J Phys Condens Matter* 23(13):135302
9. Urban DF, Bercioux D, Wimmer M, Hausler W (2011) Barrier transmission of Dirac-like pseudospin-one particles. *Phys Rev B* 84:115136
10. Korol AM, Medvid NV, Sokolenko AI (2018) Transmission of the relativistic fermions with the pseudospin equal to one through the quasi-periodic barriers. *Phys Status Solidi B* 255(9):1800046
11. Korol AM, Medvid NV (2019) Influence of the fermi velocity on the transport properties of the 3D topological insulators. *Low Temp Phys* 45(10):1117
12. Korol AM (2019) Tunneling conductance of the s-wave and d-wave pairing superconductive graphene-normal graphene junction. *Low Temp Phys* 45(5):576
13. Korol AM (2021) Supertunneling effect in graphene. *Low Temp Phys* 47(2):133
14. Setare MR, Jahani D (2010) Electronic transmission through p-n and n-p-n junctions of graphene. *J Phys Condens Matter* 22:245503
15. Setare MR, Jahani D (2010) Klein tunneling of massive Dirac fermions in single-layer graphene. *Phys B* 405:1433
16. Takahashi R, Murakami S (2011) Gapless interface states between topological insulators with opposite Dirac velocities. *Phys Rev Lett* 107:166805
17. Sen D, Deb O (2012) Junction between surfaces of two topological insulators. *Phys Rev B* 85:245402