

Supertunneling effect in graphene

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Received July 23, 2020, published online December 25, 2020

The ballistic transmission of the Dirac ultrarelativistic quasielectrons in graphene structures with the rectangular potential barrier is considered and both the single and the double-barrier structures are analyzed. Within the framework of the continuum model, the transmission coefficient of quasielectrons T is calculated depending on the parameters of the problem. It is believed that there is an electrostatic barrier, as well as the Fermi velocity barrier due to the fact that this quantity may acquire different values in the barrier and out-of-barrier regions (v_{F2} and v_{F1} , respectively) of the considered structures. It is shown that the effect of the supertunneling manifests itself in these structures which consists in the fact that under certain conditions the transmission through the structure is perfect (transmission rates $T = 1$) for the arbitrary angle of incidence of quasielectrons on the barrier. In the case of different values of the Fermi velocities in the barrier and out-of-barrier regions (the parameter $\beta = v_{F2}/v_{F1}$, which characterizes the velocity barrier, is not equal to unity), the supertunneling is observed for a certain ratio between the energy E and the barrier height U and significantly depends on β . The expression is given that determines the specified conditions for the supertunneling. In the case of equal velocities ($\beta = 1$), the supertunneling effect is observed for the quasielectron energy value E equal to half the height of the electrostatic barrier U . The analysis of the dependence of the transmission on the problem parameters is also provided.

Keywords: graphene, transmission coefficient, supertunneling.

Last years, the researchers close attention was focused on the so-called Dirac materials ([1] and references therein). These include some various and diverse substances such as the topological insulators, d -wave high-temperature superconductors, the superfluid phase ^3He , *etc.* Graphene also belongs to them (see the corresponding table in [1]) and much attention has been paid to the study of graphene as well as of the various graphene-based structures in recent years. This is due to nontrivial properties of graphene such as a linear dispersion relation for the quasiparticles, unusual quantum Hall effect, the property of chirality, the Klein tunneling, high mobility, ballistic transport, *etc.* [2]. The key value 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 [3–13]. For this purpose, a number of different methods were proposed and experimentally tested. Recently, one interesting property of some Dirac materials attracted the close attention of the researchers: this is the so-called super-Klein or omnidirectional tunneling. This effect means that, under some conditions, the transmission through the potential barrier becomes perfect, i.e., the transmission rates are equal to

unity independently on an angle of incidence of the particles on the barrier. It was first observed in the spin-1 structures (the dice lattice-based structures) and also manifested itself in some other structures (see, e.g., [10, 16]). This effect can be implemented in the photonic crystals and in the fabrication of the perfect electron focusing lens [10]. As far as we know, there were no reports on the observation of this effect in graphene by far. The aim of the present paper is to show that the effect of supertunneling can be observed in graphene.

Assume first that there is the single rectangular one-dimensional electrostatic potential barrier with the height U and width d , the interfaces coordinates being $x_l = 0$ and $x_r = d$ for the left and the right interfaces, respectively. The low-energy fermion excitations in the considered structure can be described by the following Hamiltonian (see, e.g., [2]):

$$H = -i\hbar v_F \left(\sigma_x \frac{\partial}{\partial x} + \sigma_y \frac{\partial}{\partial y} \right) + \sigma_0 U, \quad (1)$$

where v_F is the Fermi velocity, σ_x , σ_y are the Pauli matrices, and σ_0 is the unit matrix; the external potential is defined as follows:

$$U(x) = \begin{cases} 0, & x \leq 0, \\ U, & 0 < x < d, \\ 0, & x \geq d. \end{cases}$$

In the case when the Fermi velocity varies in space this Hamiltonian is not the Hermitian one [14, 15]. 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 [14, 15], the Hamiltonian of the problem can be represented as

$$H = -i\hbar\sqrt{v_F(x)} \left[\sigma_x \frac{\partial}{\partial x} \sqrt{v_F(x)} + \sqrt{v_F(x)} \sigma_y \frac{\partial}{\partial y} \right] + \sigma_0 U, \quad (2)$$

and now it has the Hermitian form [14, 15]. 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:

$$\begin{aligned} \psi_l(x, y) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ f^- \end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \begin{pmatrix} 1 \\ f^+ \end{pmatrix} e^{i(-k_x x + k_y y)}, \\ \psi_r(x, y) &= \frac{t}{\sqrt{2}} \begin{pmatrix} 1 \\ f^- \end{pmatrix} e^{i(k_x x + k_y y)}, \end{aligned} \quad (3)$$

for the barrier area we have

$$\psi_b(x, y) = \frac{a}{\sqrt{2}} \begin{pmatrix} 1 \\ g^+ \end{pmatrix} e^{i(q_x x + k_y y)} + \frac{b}{\sqrt{2}} \begin{pmatrix} 1 \\ g^- \end{pmatrix} e^{-i(q_x x - k_y y)}, \quad (4)$$

$$g^\mp = \frac{\hbar v_{F2} (\mp i q_x + k_y)}{(E - U)}; \quad f^\mp = \frac{\hbar v_{F1} (\mp i k_x + k_y)}{E};$$

$$k_x = \sqrt{\frac{E^2}{(\hbar v_{F1})^2} - k_y^2}; \quad q_x = \sqrt{\frac{(E - U)^2}{(\hbar v_{F2})^2} - k_y^2}; \quad (5)$$

$$\hbar v_{F1} k_x = E \cos \theta, \quad \hbar v_{F1} k_y = E \sin \theta, \quad \varphi = \arctan(k_y / q_x).$$

The relevant boundary conditions follows from the conservation of the probability current density [2, 14, 15] and read

$$\begin{aligned} \sqrt{v_{F1}} \psi_l(x=0^-) &= \sqrt{v_{F2}} \psi_b(x=0^+), \\ \sqrt{v_{F2}} \psi_b(x=d^-) &= \sqrt{v_{F1}} \psi_r(x=d^+). \end{aligned} \quad (6)$$

Using them we find the coefficient t in expressions for the wave functions:

$$t(E, \theta) = -2 \cos \varphi \cos \theta e^{-ik_x d} \times \left\{ [1 - \cos(\theta - \varphi)] e^{ik_x d} - [1 + \cos(\theta + \varphi)] e^{iq_x d} \right\}^{-1}. \quad (7)$$

and hence the transmission coefficient $T(E, \theta) = |t(E, \theta)|^2$.

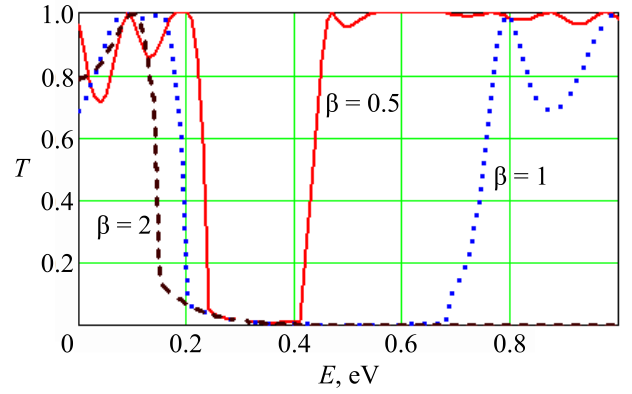


Fig. 1. Dependences of the transmission rates T on the quasi-particle energy E , $d = 10$ nm, $\theta = 0.6$ rad, $U = 0.3$ eV, $\beta = 0.5, 1, 2$.

Figure 1 shows the dependence of the transmission coefficient T on the quasi-electrons energy E (transmission spectra) for the following fixed values of the problem parameters: the barrier thickness $d = 10$ nm, the incidence angle $\theta = 0.6$ rad, the electrostatic barrier height $U = 0.3$ eV, the parameter $\beta = 0.5, 1, 2$ for the solid, dotted, dashed lines, respectively. Note firstly that all spectra show the pronounced resonant-tunneling character, which is the magnitude of T is equal to unity for some energies and $T \ll 1$ for other energies. Some particular energy values, for example, $E_+ = U/2$ ($\beta = 1$, the dotted line), $E_+ = 2U/3$ ($\beta = 0.5$, the solid line), $E_- = 2U$ ($\beta = 0.5$, the solid line), attract the special attention. The thing is that, for these energies, the effect of the supertunneling is realized: the transmission rates are equal to the maximum, $T = 1$, independently on the particle angle of incidence on the barrier. This is confirmed by Fig. 2 which demonstrates the dependence of the rates T on the incidence angle θ for different $\beta = 0.5, 1, 1.5, 2$. The parameters for all lines are as follows: $d = 10$ nm, $E = 0.2$ eV, $U = 0.4$ eV.

The horizontal line with $T = 1$ refers also to values $E = U/2$ for arbitrary U , and to some other values (e.g., for $U = 0.3$ eV, $\beta = 0.5$, $E_+ = 0.2$ eV, $E_- = 0.6$ eV used in Fig. 1). Hence, really, the effect of the supertunneling manifests itself in the graphene structures. It follows from

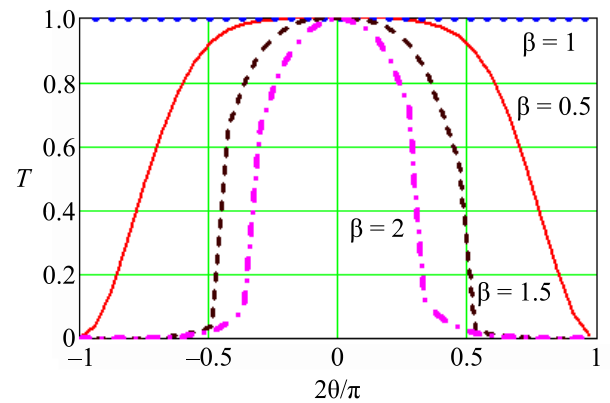


Fig. 2. Dependences of the transmission rates T on the incidence angle θ for the $d = 10$ nm, $E = 0.2$ eV, $U = 0.4$ eV, $\beta = 0.5, 1, 1.5, 2$.

the above formulae that in the case of the gapless graphene and the presence of both the velocity and the electrostatic barriers the energies for the supertunneling are determined by the following expression:

$$E_{\pm} = \frac{U}{|1 \pm \beta|} \quad (8)$$

and, hence, they essentially depend on the electrostatic barrier height U and also on the parameter β . This expression follows from the condition $q_x = k_x$ which corresponds to the leveling of the resulting barrier. Thus, the supertunneling effect takes place in the pristine graphene and it is realized for energies that are subjected to the condition (8). When the quantity β approaches unity the energy for the supertunneling E_+ tends to the value $U/2$ — as for the dice lattice case [10].

The considered structure also reveals a phenomenon similar to the Klein paradox: for the zero incidence angle, the transmission coefficient is equal to one, as shown in Fig. 2. This type of tunneling is observed regardless of β and U magnitudes.

The process of tunneling is also affected by the presence of the so-called critical angle of incidence of quasielectrons on the barrier θ_c — for quasielectrons that fall at angles greater than θ_c barrier is impermeable. The formulas above give the following expression for the critical angle

$$\theta_c = \arcsin [(E - U) / E\beta]. \quad (9)$$

So, the value of the critical angle depends on the parameters U , β and is markedly sensitive to the change of each. In the presence of the electrostatic potential ($U \neq 0$) the critical angle can exist for both $\beta > 1$ and $\beta < 1$ cases. The range of

incidence angles for which the value of $T(\theta)$ is significant as well as the value of θ_c are substantially reduced with increasing in β .

The $T(E)$ spectra are also characterized by the presence of the region where the magnitude of T is close to zero but not equal to (“energy gap”). Its presence is explained by the fact that at energies close to the top of the potential barrier, the electron wave becomes evanescent [see expressions (5)]. The “gap” width is highly dependent on the parameters β , θ increasing sharply as each of them increases. The increase in “gap” width with the growth of β is illustrated, in particular, by Fig. 1 (compare the solid and the dotted curves). Note that the incidence angle exceeds the critical one for the dashed curve in Fig. 1 so that the value of T tends to zero for large energies.

In addition to resonances related to the supertunneling phenomenon, there are a number of resonance peaks of a different origin (see, e.g., Fig. 1). Namely, these are the Fabry–Perot-type resonances whose energy position is determined by the formula

$$d \sqrt{\frac{(E - U)^2}{(\hbar v_{F2})^2} - k_y^2} = n\pi, \quad (10)$$

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

The phenomenon of the supertunneling occurs also in graphene-based double-barrier resonant tunneling structure (DBRTS). Assume that barriers are symmetric with the same thickness d and the quantum well width is equal to w . The expression for the transmission rates in this case can be found in a manner analogous to the SBRTS case and it reads

$$T_2 = \cos^2 \theta \cos^2 \varphi / \left\{ \cos^2 \theta \cos^2 \varphi + \left(2 \sin(q_x d) (\sin \theta - \sin \varphi) [(\sin \theta \sin \varphi - 1) \sin(q_x d) \sin(k_x w) + \cos \theta \cos \varphi \cos(q_x d) \cos(k_x w)] \right)^2 \right\}. \quad (11)$$

It follows from this formula that the energies of the supertunneling E_{\pm} are determined by the same expression as in the case of the single barrier RTS (8). Other barrier resonances (Fabry–Perot-type) also retain their energy positions (location on the energy axis). The dependence of the transmission rates T_2 on energy E is depicted in Fig. 3 for the following parameters: $d = 10$ nm, $w = 25$ nm, $U = 0.3$ eV, $\varphi = 0.6$ rad, $\beta = 0.5, 1, 2$.

There are a number of new resonances with high values of the coefficient T — these are the well-induced resonances. Their number increases with the quantum well widening. Besides, there are special resonances in the transmission spectra. Their energy positions are determined by the following equation:

$$(1 - \sin \varphi \sin \theta) \operatorname{tg}(k_x w) \operatorname{tg}(q_x d) = \cos \varphi \cos \theta. \quad (12)$$

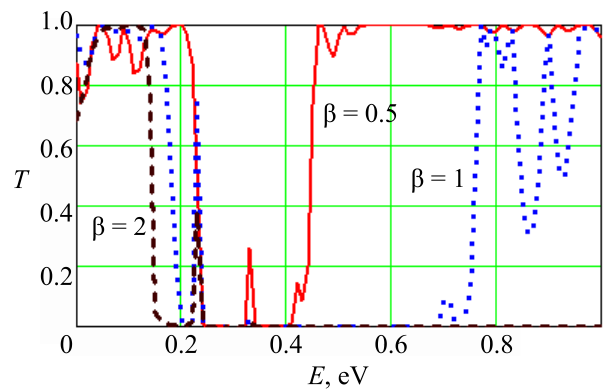


Fig. 3. Dependences of the transmission rates T on the quasi-particle energy E for the DBRTS. The parameters are as follows: $d = 10$ nm, $w = 25$ nm, $U = 0.3$ eV, $\varphi = 0.6$ rad, $\beta = 0.5, 1, 2$.

In the general case, there may be a large variety of different configurations of the spectra due to the well-induced resonances. Varying the problem parameters it is possible to obtain very different spectra including the symmetric ones. The tunneling spectra in the DBRTS in general are irregular (nonperiodic) over the entire energy scale, comprising the part where they are periodic in the SBRTS. By selecting certain sets of the problem parameter values it is possible to achieve the full periodicity of the spectra. This is possible if the number $\beta w \cos \varphi / (2d \cos \theta)$ is the rational one; if it is an irrational number then the spectra $T(E)$ are irregular. The location of the spectral resonances (peaks) may not be fully random even in those parts of the spectrum where at the first glance the resonance peaks are quite chaotic.

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Ефект супертунелювання в графені

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Розглянуто балістичну трансмісію ультрарелятивістських квазіелектронів Дірака в графенових структурах із прямокутним потенціальним бар'єром та проаналізовано як одно-, так і двобар'єрну структури. В рамках континуальної моделі розраховано коефіцієнт трансмісії квазіелектронів T в залежності від параметрів задачі. Вважається, що існує електростатичний бар'єр, а також бар'єр швидкості Фермі, обумовлений тим, що ця величина має різні значення в бар'єрній та позабар'єрній областях розглянутих структур (v_{F2} та v_{F1} відповідно). Показано, що в даних структурах має місце ефект супертунелювання, який полягає в тому, що за певних умов трансмісія крізь структуру є ідеальною (коефіцієнт трансмісії $T = 1$) для будь-якого кута падіння квазіелектронів на бар'єр. У разі різних значень швидкості Фермі в бар'єрній та позабар'єрній областях (параметр $\beta = v_{F2}/v_{F1}$, який характеризує бар'єр швидкості, не дорівнює одиниці) ефект супертунелювання спостерігається при певному співвідношенні між енергією квазіелектронів E й висотою електростатичного бар'єра U та істотно залежить від β . Наведено вираз, яким визначається зазначена умова для супертунелювання. Якщо $\beta = 1$, то супертунелювання має місце при енергії, що дорівнює половині висоти електростатичного бар'єру. Також проведено аналіз залежності коефіцієнта трансмісії від параметрів задачі.

Ключові слова: графен, коефіцієнт трансмісії, супертунелювання.