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PECULIARITIES OF THE MOTION OF THE PSEUDORELATIVISTIC DIRAC QUASIPARTICLES IN THE ALPHA-T_3 MODEL WITH THE STEP-LIKE BARRIER

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ABSTRACT

Within the continuous approach, the transmission coefficient T of the Dirac quasielectrons through a step-like potential barrier in the α-T_3 model is calculated and analyzed. It is believed that the degree of coupling of the central atom with the atoms in the vertices of the hexagonal lattice is characterized by the parameter α, which can acquire values from zero to one. Particular attention is given in the work to intermediate values of α, since, it is known from the literature, that they are important for observing a lot of physical phenomena. The wave functions as well as the transmission ratio are sought by the Dirac type equation. The Hamiltonian of the system is represented by a spinor of 9 components, which is expressed, in particular, by the parameter α. The transmission coefficient is found by means of matching of wave functions at heterojunctions.

In particular, it is found that there is a range of problem parameters, such as the height of the electrostatic barrier *U*, the energy of the quasielectrons *E*, the ratio of the Fermi velocities in the barrier and out-of-barrier areas β, in which the value of the transmission coefficient reaches maximum, that is, it is close to unity for α values close to unity. In this area, the dependence of the transmission coefficient on the value of α is weak. When the value of α becomes exactly equal to one, then the value of the transparency coefficient reaches the absolute maximum, that is, one. For the zero angle of incidence of quasiparticles on the barrier, the Klein paradox phenomenon is observed, i.e, the quantum transparency of the system is perfect, and this is right for any values of the parameters α, β, *U*, *E*. For certain ratios of particle energy *E*, the barrier height *U* and the magnitude of β there is the supertunneling phenomenon, which is that under these conditions the transmission coefficient is equal to one independently of the angle of incidence of the particles on the barrier. Characteristic of the transmission spectra *T*(*E*) is also the presence of a critical angle of incidence and a gap of energies.

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ОСОБЛИВОСТІ РУХУ ПСЕВДОРЕЛЯТИВІСТСЬКИХ ДІРАКІВСЬКИХ КВАЗІЧАСТИНОК В АЛЬФА-T_3 МОДЕЛІ ІЗ СХОДИНКОПОДІБНИМ БАР'ЄРОМ

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У рамках континуального підходу розраховано і проаналізовано коефіцієнт трансмісії T діраківських квазіелектронів крізь сходинкоподібний потенціальний бар'єр в α-T_3 моделі. Вважається, що ступінь зв'язку центрального атома з атомами у вершинах гексагональної гратки характеризується параметром α, який може набувати значення від нуля до одиниці. Особливу увагу приділено проміжним значенням α, оскільки, як відомо з літератури, вони є важливими для спостереження низки фізичних явищ. Хвильові функції, а також коефіцієнт трансмісії визначено за допомогою рівняння діраківського типу. Гамільтоніан системи представлено спінором із дев'яти компонентів, які виражаються, зокрема, через параметр α. Коефіцієнт трансмісії знайдено за допомогою зшивання хвильових функцій на гетеромежах.

З'ясовано, зокрема, що існує область параметрів задачі, таких як висота електростатичного бар'єру U, енергія квазіелектрона E, відношення швидкостей Фермі в бар'єрній і позабар'єрній областях β, в якій значення коефіцієнта трансмісії досягає максимуму, тобто наближається до одиниці, для близьких до одиниці значень α. В цій області залежність коефіцієнта трансмісії від величини α є слабкою. Коли величина α стає точно рівною одиниці, то і значення коефіцієнта прозорості досягає абсолютного максимуму, тобто одиниці. Для нульового кута падіння квазічастинок на бар'єр спостерігається явище клейнівського парадоксу, тобто квантова прозорість системи є ідеальною, і це справедливо для будь-яких значень параметрів α, β, U, E. Для певних співвідношень енергії частинок E, висоти бар'єру U і величини β має місце явище супертунелювання, яке полягає в тому, що для заданих умов коефіцієнт трансмісії дорівнює одиниці незалежно від кута падіння частинок на бар'єр. Характерним для трансмісійних спектрів T(E) є також наявність критичного кута падіння та забороненої зони енергій.

Ключові слова: *α-T_3 модель, сходинкоподібний бар'єр, спектри трансмісії.*

Introduction. Some modern physical structures can be conveniently described using the so-called α-T_3 model [1—8]. This model can rightly be attributed to a new class of objects that have received the name of Dirac materials in recent years [9]. These include very different objects in their structure, in particular the low and high-temperature d-wave superconductors, superfluid phases 3He, graphene, two- and three-dimensional insulators etc. [9]. The key concept that unites these different objects is a linear dispersion relation that describes the low-energy excitations of the quasiparticles. Due to the fact that the Dirac materials have a number of non-trivial, interesting properties, they are actively studied in the last time. Under low energies, the quasiparticle states of the Dirac materials are described by a massless Dirac equation in one or two dimensions, analogous to the equation for the quasielectrons in graphene. The dispersion relation for the Dirac particles relates to a cone in the three-dimensional case. Some properties of the quasiparticle states are expressed in terms of topologically invariant quantities and, importantly, are protected from the influence of moderate perturbations due to the symmetry of inversion of time in the corresponding Hamiltonian.

The α-T_3 model is an intermediate structure between a dice lattice and graphene. It is characterized by the parameter α, which determines the coupling strength between the central atom of the hexagonal lattice and the atoms in the hexagon vertices [1—8]. It is clear that different values of α correspond to different physical states of the α-T_3 model and it was successfully applied to various physical structures [1—8].

At the same time, it is known that the characteristics of structures based on Dirac materials are significantly influenced by the difference in the values of the Fermi velocity in different parts of the structure [10—19]. A lot of various structures with non-equal Fermi velocities in different areas of the given structure were studied in last years. They comprise the graphene based single- and double-barrier structures, various types of superlattices including the quasiperiodic ones, superconducting junctions, structures based on the topological insulators etc. [10—19].

Motivated by the above considerations, in this paper, we study the ballistic transmission of quasielectrons through a step-like potential barrier in the α-T_3 model, and show that it depends strongly on the relation between the parameters α and β, where β is equal to the ratio of the Fermi velocities in the barrier and out-of-barrier areas. By changing the values of the parameters α and β, one can flexibly control the transmission properties of the structure under consideration within a wide range.

Model and Formulae. The Dirac-like equation for the considered model can be represented as follows [1—8]

$$\begin{pmatrix} 0 & f\cos\varphi & 0 \\ f^*\cos\varphi & 0 & f\sin\varphi \\ 0 & f^*\sin\varphi & 0 \end{pmatrix}\psi + UI_0\psi = E\psi \quad (1)$$

where U is the external potential which corresponds to the rectangular barrier and is equal to

$$U(x) = \begin{cases} 0, & x \le 0 \\ U, & x > 0 \end{cases} \quad (2)$$

in different areas of the given structure; I_0 is the identity matrix.

The quantity f in (1) is equal to

$$f = \nu_F\left(k_x - ik_y\right) \quad (3)$$

where k_x, k_y are the quasi-momentum components, v_F the Fermi velocity.

For our purpose it is sufficient to take into consideration only one K valley in the hexagonal Brillouin zone. The quantities v_F and k_x acquire different values in the barrier and out-of-barrier areas. The parameter φ is introduced for convenience: $\varphi = \mathrm{arctg}\alpha$, α is a parameter showing the coupling strength of the central atom with the atom at the hexagon vertices; for the dice lattice $\alpha = 1$, for graphene $\alpha = 0$.

The eigenfunctions in the equation (1) can be represented as follows:

$$\Psi_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} \cos\varphi e^{i\theta} \\ 1 \\ \sin\varphi e^{-i\theta} \end{pmatrix} e^{ik_x x} e^{ik_y y} + \frac{r}{\sqrt{2}}\begin{pmatrix} -\cos\varphi e^{i\theta} \\ 1 \\ -\sin\varphi e^{i\theta} \end{pmatrix} e^{-ik_x x} e^{ik_y y} \tag{4}$$

where θ, φ are the angle of incidence and the refraction angle respectively, the quasimomentums in the out-of-barrier area kx and in the barrier area qx are equal to:

$$k_x = \sqrt{E^2 - k_y^2};\; q_x = \sqrt{\frac{(U-E)^2}{\beta} - k_y^2};$$
$$tg\varphi = \frac{q_y}{q_x};\; q_y = k_y \tag{5}$$

the linear dispersion relation is used and the units with $v_{FI} = 1$; $\hbar = 1$ are adopted.

Using the appropriate matching conditions [20, 21] we can deduce the expression for the transmission coefficient T:

$$T = 4\cos^2\theta\cos^2\varphi / f_p^2$$
$$f_p = 2 - 2\cos(\theta+\varphi) - \sin^2(2\varphi)(\sin\theta + \sin\varphi)^2 \tag{6}$$

Results and Discussion. The most important and at the same time characteristic feature of the presented graphs is the presence of resonance values T=1 in them, which testify to the perfect transparency of this structure for the certain energies. As can be deduced from the formulas above, the values of the energies E_l for which perfect transparency holds are subordinated to the formula

$$E_l = \frac{U}{|1 \pm \beta|}$$

that is, these values are essentially dependent on the parameters U and β and are independent of α. As shown in the following Fig. 1 for the dependence of T on the angle of incidence θ, the energy $E\pm$ corresponds to the phenomenon of the supertunneling, which is that under these conditions the transmission coefficient is equal to one independently from the angle of incidence of the particles on the barrier.

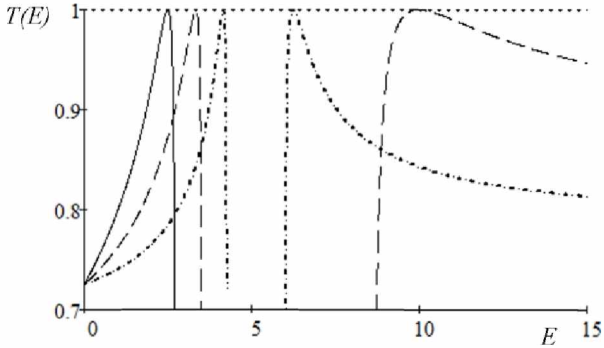

Fig. 1. Plot of $T(E)$ function for the following set of the problem parameters: $U = 5$, $\alpha = 0$, $\theta = 1.3$ for all curves, $\beta = 0.2, 0.5, 1$ for the dashed and dotted, dashed and solid lines respectively

Thus, an important conclusion can be made: in the system under consideration, it is possible to create conditions for the realization of the phenomenon of the super-tunneling.

In the general case, an increase in the parameter α leads to an increase in T, which is clearly visible both as a function of $T(E)$ (Figs. 1, 2) and as a function of $T(\theta)$ (Fig. 3a, b).

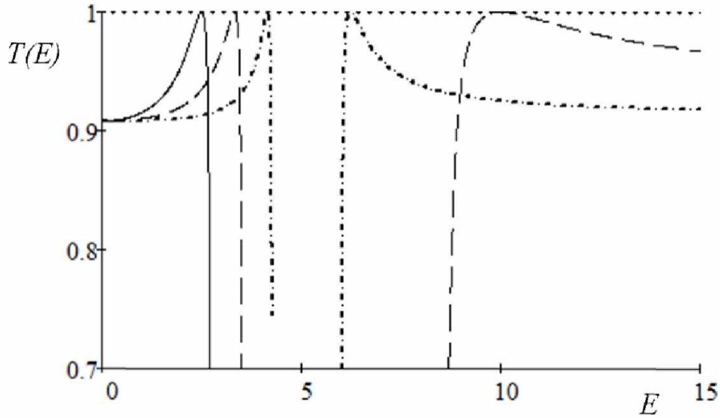

Fig. 2. Plot of the $T(E)$ function for the following set of the problem parameters: $U = 5$, $\alpha = 1$, $\theta = 1.3$, $\beta = 0.2, 0.5, 1$ for the dashed and dotted, dashed and solid lines respectively

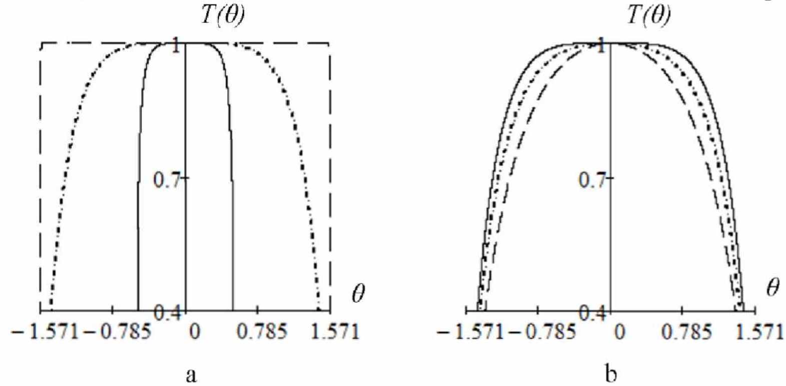

Fig. 3. a. T vs θ dependence, other parameters are as follows: $E = 2$, $U = 3$, $\beta = 5$ for all the curves, $\alpha = 0, 0.5, 1$ for the solid, dashed and dashed and dotted lines respectively;
b. T vs θ dependence, other parameters are as follows: $E = 2$, $U = 3$, $\beta = 0.1$ for all the curves, $\alpha = 0, 0.5, 1$ for the solid, dashed and dashed and dotted lines respectively

The dependence of T on the actual parameter α can be traced using Fig. 4. It is seen that T is weakly dependent on α over the entire range of change α, see also Fig. 3. a, b. At the same time, T strongly depends on θ, see Figs 3. a, b falling sharply with increasing θ until the angles θ exceeds the critical angle θ_c, resulting in a completely opaque barrier. And for small θ, the value of T is large.

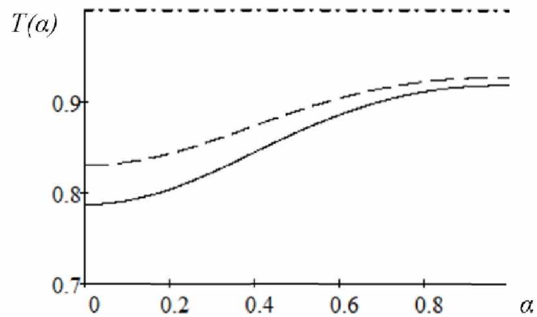

Fig. 4. Graph of the $T(\alpha)$ dependence, other parameters are as follows: $U = 3$, $E = 2$, $\theta = 1$, for all curves, $\beta = 0.2, 0.5, 1$ for the dashed, dashed and dotted, and solid lines respectively

For the same reason, T also falls sharply with increasing β, which is explained by the formula for the critical angle θ_c that we obtained from the Snell's law. The dependence of T on U has the form similar to the dependence of $T(E)$; this is quite natural since the quantities E and U are included in the formula for T in a symmetrical manner.

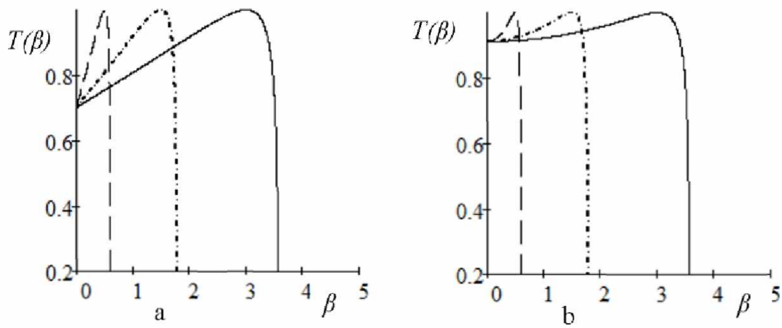

Fig. 5. a. T vs β dependence, other parameters are as follows: $E = 2$, $\theta = 1$, $\alpha = 1$, with solid lines of $U = 8$, the dotted line of $U = 3$, the dashed line of $U = 1$;

b. T vs β dependence, other parameters are as follows: for solid line $U = 8$, the dotted line $U = 3$, the dashed line $U = 1$, $E = 2$, $\theta = 1$, $\alpha = 0$

Analyzing the dependence of the transmission spectra on the parameter β presented in Figs. 5. a, b (the parameters for these figures are as follows: $E = 2$, $\theta = 1$ for both figures, $\alpha = 1$ and $\alpha = 0$ for Figs. 5. a and 5. b, respectively, with solid lines the value of $U = 8$, the dotted $U = 3$, the dashed $U = 1$), note the following features: 1) the dependence of $T(\beta)$ is weak for small values of β ($\beta<1$); 2) curves $T(\beta)$ are characterized by the presence of a maximum corresponding to the phenomenon of supertunneling; 3) characteristic of both figures is a sharp decrease in the value of T with increasing and exaggerating parameter β of the critical value β_c. This means that if, for example, we fix all parameters except the angle of incidence θ, then a very sharp decrease in T will be observed when approaching θ to the critical value θ_c.

Conclusions

Transmission properties of single-barrier structure based on α-T_3 model are considered in the paper. It is believed that the barrier is sharp and has a rectangular shape. The physical origin of the barrier is assumed to be electrostatic, but it is taken into account that the Fermi velocities in the barrier and non-barrier areas have different values and are referred to in the literature as the Fermi velocity barrier. The parameter α in this model can take values from zero to one, moreover the case $\alpha = 0$ corresponds to graphene and $\alpha = 1$ to the dice lattice. Particular attention is given in the work to intermediate values of α, since, as is known from the literature, they are important for observing of a lot of physical phenomena. The wave functions as well as the transmission ratio are obtained by the Dirac type equation. The Hamiltonian of the system is represented by a spinor of 9 components, which is expressed, in particular, by the parameter α. The transmission coefficient is deduced by means of matching of wave functions at the heterojunctions.

The obtained spectra show a pronounced dependence on an angle of incidence of pseudo-relativistic Dirac quasiparticles on the barrier of the structure under consideration. In particular, for the zero incidence angle, there is a perfect penetration of particles through the barrier for any values of the parameters α, β, as well as of the barrier height and thickness, that is, an effect similar to the Klein paradox is realized. Instead, for certain energies the quasiparticles we observe the effect of supertunneling, which is that for these energies the barrier of the system becomes absolutely quantum-transparent for any angle of incidence of the particles on the barrier.

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