WAVE PACKET DYNAMICS IN A MONOLAYER GRAPHENE AT THE PRESENCE OF ELECTRIC FIELD

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In this work we study the space-time evolution of electron wave packet moving in monolayer graphene placed in potential field, potential barrier, and wells. In particular, we describe and visualize the effect of additional splitting and interference in the process of Klein tunneling [1]. The Klein tunneling is one of the most important manifestations of the relativistic Dirac spectrum in graphene [2]. In this process an electron crosses a gap between two bands, which is a classically forbidden area, and transforms from an electron to a hole, or vise versa. At first time the effect of Klein tunneling on conductance in a graphene sheet in the ballistic regime was investigated in a series of works [2],[3].

Graphene is a single layer of carbon atom densely packed in a honeycomb lattice. The two-dimensional Hamiltonian describing its band structure has the form [4]

$$\widehat{H} = \widehat{H}_0 + \hat{I}U(x,y) = v_F\left(\hat{p}_y\hat{\sigma}_x + \hat{p}_x\hat{\sigma}_y\right) + \hat{I}U(x,y), \tag{1}$$

where v_F is the Fermi velocity, $\widehat{\vec{p}}$ is the momentum operator defined with respect to the centre of the valley centered at the corner of the Brillouin zone, $U(x,y)$ is the potential energy, $\hat{I}$ is a unit matrix. Here Pauli matrices $\hat{\sigma}_i$ operate in the space of the electron amplitude on two sites (A and B) in the unit cell of a hexagonal crystal, the internal degree of freedom playing a role of a pseudospin.

We represent the initial electron wave function by Gaussian wave packet having the width d and nonvanishing average momentum $p_{0x} = \hbar\, k_{0x}$,

$$\psi(\vec{r},0) = \frac{1}{d\sqrt{\pi(|c_1|^2+|c_2|^2)}}\exp\left(-\frac{r^2}{2d^2} + ik_{0x}x\right)\begin{pmatrix}c_1\\c_2\end{pmatrix}, \tag{2}$$

where coefficients c_1 and c_2 determine the initial pseudospin polarization, the packet width d is much greater than the lattice period and consequently $\psi(\vec{r},0)$ is smooth enveloping function. We suppose that Fermi level is located in the valence band and consider the problem in a one electron approximation.

For a numerical solution of the equation

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\\psi_2\end{pmatrix} = \widehat{H}\begin{pmatrix}\psi_1\\\psi_2\end{pmatrix} \tag{3}$$

we adapt here a finite difference method described in [4] for solution of the two-dimensional massless Dirac equation. We use Crank-Nicholson scheme with Caley transformation of evolution operator.

Below we discuss the simple case when the initially localized wave packet Eq.(2) moves in a uniform electric field with potential $V(x) = -e\mathcal{E}x$. The results of numerical calculations for electron probability density (see Fig. (a)) and pseudospin density (see Fig. (b)) are presented below for the initial wave packet (2) with polarization $c_1 = 1$ and $c_2 = 1$ and average momentum k_{ox}. One can show that this initial wave packet can be considered as mainly a superposition of positive energy states of the Hamiltonian $\widehat{H}_0$. As one can see from Fig. (a) the packet moving in the direction of vector $\vec{\mathcal{E}}$ parallel to x axis splits into parts. The splitting takes place at the point x_c where $k_x = 0$. At this point one part which is a superposition of the states with small k_y demonstrates Klein-like tunneling from the conduction band to the valence band. The right and left reflected parts are the superposition of the states with $k_y > 0$, $k_y < 0$ correspondingly. In Fig. (b) we illustrate the evolution of the component of the pseudospin density: $s_x(x,y,t) = 2Re(\psi_1{}^*\psi_2)$. If at $t = 0$ this component had the positive sign then at moment $t = 90$ *(in the units of d/u)* the reflected and transmitted parts get opposite pseudospin polarization. This is a result of that the reflected and transmitted part are superpositions of states with different chirality. If should be noted that the wave packet with the same initial average momentum k_{0x} and polarization $c_1 = 1$ and $c_2 = -1$ which is a superposition of negative energy states in a uniform

electric field propagates in opposite direction, and the tunneling takes place from the band E^- to the band E^+.
For the arbitrary pseudospin polarization when the wave packet can be considered as a superposition of the positive- and negative- energy states of Hamiltonian $\hat{H}_0$, the wave packet evolution is directly related to the Klein tunneling between two bands. In this case the reflected parts of the wave packet moving in opposite directions interfere that result in the new type of Zitterbewegung oscillation of the average packet coordinates and pseudospin polarization at the presence of electric field.

In our presentation we shall consider also the wave packet tunneling thought the potentials barriers and wells.

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References

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Figure

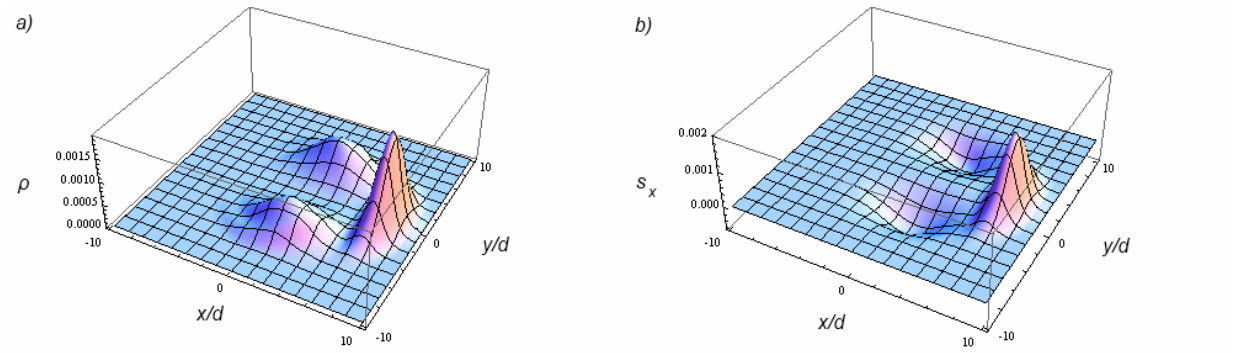

Figure caption

The electron probability density $\rho(x,y,t)) = |\psi_1|^2 + |\psi_2|^2$ *(a) and* pseudospin *density* $s_z(x,y,t)$ *(b) for initial wave packet Eq.(2) with* $c1 = 1$ *and* $c2 = 1$ *for* $k_{0x}d = 2$*, at time* $t = 90$ *(in units of* d/u*). The calculation was performed for* $d = 20\,nm$ *and for electric field* $E_x = u\hbar/3ed^2$ *which corresponds to the amplitude* $E_x = mV/cm$*.*