Semiclassical analysis of tunneling in graphene in the presence of a smoothly inhomogeneous external electromagnetic field

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I study the influence of a static magnetic field $\boldsymbol{B}$ on the tunneling of the Dirac fermions in graphene monolayer through an external electrostatic potential barrier U. The carriers are assumed to have a low energy, their dispersion relation can be approximated by a cone and their wave function obeys the Dirac equation.

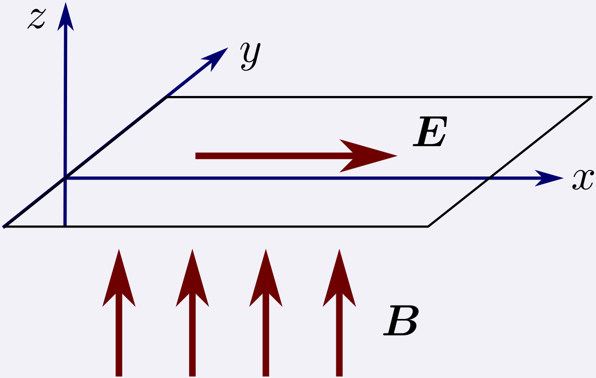
The fields are assumed to be smoothly inhomogeneous.

Wave functions are found in semiclassical approximation by applying the turning point theory for systems of differential equations.

Reflection and transmission coefficients (their moduli and phases)are obtained.

Graphene is immersed in the external stationary fields

Graphene sheet. Fields



Fields smoothly depend on one variable x, $\boldsymbol{A} = (0, A_y(x), 0)$,

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}, \quad \boldsymbol{B} = (0, 0, B(x)), \quad \boldsymbol{E} = -\nabla U(x).$$

Governing equations

The wave function of the fermion (electron or hole) $\boldsymbol{\Upsilon}(\boldsymbol{r}, t)$, $\boldsymbol{r} = (x, y)$, obeys the 2D Dirac equation

$$i\hbar \frac{\partial}{\partial t} \boldsymbol{\Upsilon} = \hat{H}(\hat{\boldsymbol{p}}, \boldsymbol{r}) \boldsymbol{\Upsilon}, \quad \hbar \ll 1,$$

here the Hamiltonian reads

$$\hat{H}(\hat{\boldsymbol{p}}, \boldsymbol{r}) = v_F \hat{\boldsymbol{\sigma}} \cdot (\hat{\boldsymbol{p}} + e\boldsymbol{A}(\boldsymbol{r})) + U(\boldsymbol{r}),$$

where $\hat{\boldsymbol{p}} = -i\hbar\nabla$ is a momentum operator,
v_F is the Fermi velocity, e is the electron charge, $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_1, \hat{\sigma}_2)$,
the Pauli matrices $\hat{\sigma}_1$ and $\hat{\sigma}_2$ read

$$\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

We assume that $\hbar \ll 1$ and obtain the semiclassical solution, which reads

$$\mathbf{\Psi}(x;\hbar) \approx \mathbf{\Phi}(x)\exp\left\{\frac{i}{\hbar}\left(\int^{x} p_x(x')\,dx' + p_y y - \mathcal{E}t\right)\right\},$$

$$p_x = \sqrt{v_F^{-2}(\mathcal{E} - U(x))^2 - (p_y + eA_y(x))^2},$$

here $\mathcal{E}$ is an energy of the carrier, $p_y = const$ is a y - component of its momentum.

If $p_x(x)$ is real, then x belongs to the classically allowed region and $\mathbf{\Psi}(x;\hbar)$ corresponds to the carrier, which runs without reflection.

If $p_x(x)$ is imaginary, then x belongs to the classically forbidden region .

If $p_x(\varkappa) = 0$, then $x = \varkappa$ is a turning point, in the vicinity of which the semiclassical approach fails, the reflection can arise.

The condition of applicability reads

$$\frac{(p_x)_{typical}(x-x_0)}{\hbar} \gg 1, \quad r \equiv \frac{|\mathcal{E}-U(x)|_{typical}(x-x_0)}{v_F \hbar} \gg 1.$$

If $|\mathcal{E}-U(x)|_{typical} \sim 0.1eV$, the length of transition is $(x-x_0) \sim 70nm$, then $r = 10$. Magnetic field should be less than 1 T.

We are interested in studying the scattering process, i.e., the coefficients of reflection and transmission of carriers as functions of external fields.

To do this we find the turning points, in the vicinity of which the semiclassical fails. The behavior of turning points meets conditions of the paper

V. V. Fialkovsky, M. V. Perel, Mode transformation for a Schrödinger type equation: Avoided and unavoidable level crossings, *Journal of Mathematical Physics*, 61, 043506 (2020).

where the coefficients of reflection and transmission were found for equations in the general form.

I. V. Cheianov, V. I. Fal'ko, Selective transmission of Dirac electrons and ballistic magnetoresistance of n- p junctions in graphene, *Physical Review B*, **74**(4), 041403 (2006).

K. J. A. Reijnders, T. Tudorovskiy, and M. I. Katsnelson, Semiclassical theory of potential scattering for massless Dirac fermions, *Ann. Phys.*, **333**, 155B—197 (2013).

V. Zalipaev, C. M. Linton, M. D. Croitoru, and A. Vagov, Resonant tunneling and localized states in a graphene monolayer with a mass gap, *Phys. Rev. B* **91**, 085405 (2015).

V. V. Fialkovsky, M. V. Perel, Mode transformation for a Schrödinger type equation: Avoided and unavoidable level crossings, *Journal of Mathematical Physics*, **61**, 043506 (2020).

No magnetic field. Dirac eq. versus Schroedinger eq.

Let $U(x)$ be a smooth monotonne increasing function and $\boldsymbol{B} = 0$. The momentum reads

$$p_x = \pm\sqrt{(\mathcal{E} - U(x))^2 - p_y^2}.$$

If $p_y = 0$, the single turning point $\varkappa_{\mathcal{E}}$ satisfies the equation

$$\mathcal{E} - U(\varkappa_{\mathcal{E}}) = 0.$$

All x belong to the classically allowed region, because $p_x = \pm|\mathcal{E} - U(x)|$.

We compare $\boldsymbol{\Psi}(x)$ with the solution ψ^s of the Schroedinger equation

$$-\frac{\hbar^2}{2m}\Delta\psi^s + U(x)\psi^s = \mathcal{E}\psi^s, \quad \psi^s(x;\hbar) \approx \phi^s(x)e^{\frac{i}{\hbar}\left(\int\limits_{x_0}^{x} p_x^s(x')\,dx' + p_y y - \mathcal{E}t\right)},$$

$$p_x^s = \pm\sqrt{\mathcal{E} - U(x) - p_y^2}.$$

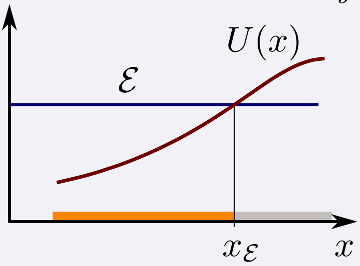
All $x > \varkappa_{\mathcal{E}}$ belong to the classically forbidden region, because $p_x = \pm\sqrt{\mathcal{E} - U(x)}$.

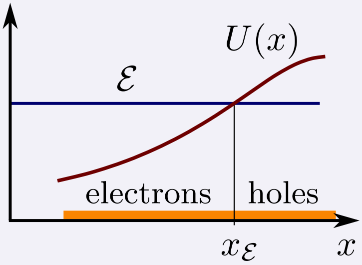
$$p_x^s = \pm\sqrt{\mathcal{E} - U(x) - p_y^2}, \quad p_x = \pm\sqrt{(\mathcal{E} - U(x))^2 - p_y^2}.$$

Classically allowed (forbidden) regions are marked by orange (grey).

Schroedinger equation | **Dirac equations**

$p_y = 0$





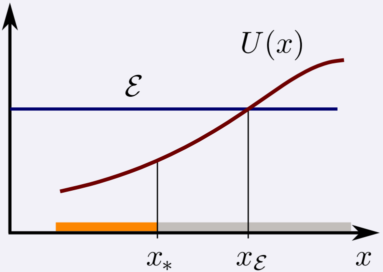
The full reflection occurs near $\varkappa_{\mathcal{E}}$.

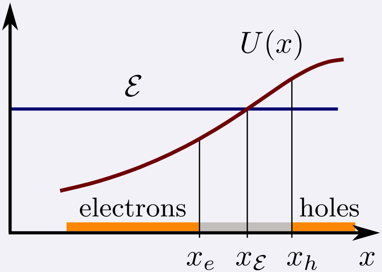
The full transmission takes place. (The Klein tunneling)

$$p_x^s = \pm\sqrt{\mathcal{E} - U(x) - p_y^2}, \quad p_x = \pm\sqrt{(\mathcal{E} - U(x))^2 - p_y^2}.$$

Schroedinger equation | **Dirac equations**

$p_y \neq 0$





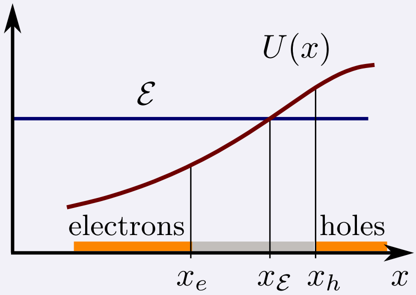
The point of reflection is shifted

The classically forbidden zone arises. Reflection occurs.

Non-zero magnetic field

$$p_x = \pm\sqrt{v_F^{-2}(\mathcal{E} - U(x))^2 - (p_y + eA_y(x))^2}.$$

Dirac equations



The turning points are shifted.

None-zero magnetic field

Semiclassical wave function of electrons read

$$\mathbf{\Psi}(x;\hbar) \approx \mathbf{\Phi}(x) \exp\left\{ \frac{i}{\hbar} \left(\int^{x} p_x(x')\, dx' + p_y y - \mathcal{E} t \right) \right\},$$

$$p_x = \pm\sqrt{v_F^{-2}(\mathcal{E} - U(x))^2 - (p_y + eA_y(x))^2},$$

$$\mathbf{\Phi}(x) = \alpha \frac{\boldsymbol{\varphi}(x)}{|2p_x(\mathcal{E} - U(x))|^{1/2}} \exp\left\{ \frac{i}{2} \arccos \frac{v_F(p_y + eA_y(x))}{|\mathcal{E} - U(x)|} \right\},$$

$$\boldsymbol{\varphi} = \begin{pmatrix} i(p_y + eA_y(x)) - p_x \\ U(x) - \mathcal{E} \end{pmatrix},$$

Direction of propagation is determined by the sign

$$\mathrm{sgn}(j_x) = \mathrm{sgn}(p_x(\mathcal{E} - U(x))).$$

Let the asymptotics of the solution read in the electron and hole regions:

$$\boldsymbol{\Psi} \approx \boldsymbol{\Psi}_{e+} + r\,\boldsymbol{\Psi}_{e-}, \qquad \boldsymbol{\Psi} \approx t\,\boldsymbol{\Psi}_{h+},$$

where r and t are the reflection and transmission coefficients, respectively.

$$r = -\sqrt{1 - e^{-2\pi|\nu|}}, \quad t = e^{-\pi|\nu|}.$$

$$\nu = -i\left(\frac{p_y + eA_y(x_{\mathcal{E}})}{\sqrt{\hbar}}\right)^2 \frac{v_F}{2U'(x_{\mathcal{E}})} \left(\frac{(U'(x_{\mathcal{E}})/v_F)^2}{(U'(x_{\mathcal{E}})/v_F)^2 - e^2B^2(x_{\mathcal{E}})}\right)^{3/2}.$$

$$A_y(x_{\mathcal{E}}) = B(x_{\mathcal{E}} - x_0)$$

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