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Interband transmission in armchair graphene ribbons with a step-like profile of potential energy: Relevance to Klein's tunneling

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Three principal results concerning graphene-based wires and their ambipolar behavior are presented. First, it is the exact expression of the transmission coefficient for armchair graphene wires described by the tight-binding Hamiltonian with the step-like change U of site energies. Second, the exact relation between the energy of incident electrons or holes and potential U at which there is no backscattering for the given mode of the transverse motion. Third, the range of relevance of Klein's formula describing the motion of relativistic particles in the same potential profile is established. Analysis of newly derived results shows that physics of interband transitions at constant energy in graphene wires is richer than it was believed.

1 Introduction In the rapidly growing literature on graphene electronic properties, "Klein tunneling" is a frequently used term. It refers to the formula obtained by Oskar Klein 80 years ago [1] to describe the free motion of relativistic particles, when the potential energy changes in a step-like manner, as shown in Fig. 1a (see also Ref. [2] for related references). The applicability of the Dirac equation to the description of graphene has a very solid theoretical background that has been used to investigate various aspects of graphene physics [3, 4], in particular, the coherent transport of charge carriers in graphene structures [5–8]. It is well known that this approach is valid if the conditions of long wave approximation and closeness to the neutrality point are fulfilled. These requirements are not always met. For example, nanowide graphene ribbons and large gate voltages cannot be described in the framework of "relativistic" approximation.

This communication is focused on the transmission of electrons or holes through the step potential of arbitrary magnitude U in an armchair graphene ribbon (aGR) of arbitrary width. The analysis is based on the tight-binding model that reasonably describes π electron subsystem without the above-mentioned restrictions. For all possible interband transitions at constant energy, which are illustrated in Fig. 1b, the exact expression of transmission probability is obtained in an explicit form. The Klein formula is re-derived directly from exact model results for wide aGRs and a limited range of step potential and tunneling energies. The possibility of transmission without backscattering is thoroughly examined. It is shown that the origin and manifestations of this effect in narrow aGRs are essentially different from predictions made for infinite systems [5–8].

2 Transmission coefficient The transmission coefficient T can be obtained by finding the solution of Lippman–Schwinger equation adopted for the given model [9]. With the reference to notations explained in Fig. 1, the wave function amplitudes to the left (L) and right (R) from the step, can be represented as $\sqrt{2/(\mathcal{N}+1)}\sin(m\xi_j)\psi_{n,\alpha}^{j\mathrm{L(R)}}$, $\alpha = l, r$, $\xi_j = \pi j/(\mathcal{N}+1)$, $j = 1,2,\ldots,\mathcal{N}$. Due to model simplicity, there is no $j \to j'$ transitions so that the problem reduces to calculation of sum $T = \sum_{j=1}^{\mathcal{N}} T_j$, where

$$T_j = \frac{\overline{v}_j}{v_j}\left|\psi_{n,l}^{j\mathrm{R}}\right|^2, \tag{1}$$

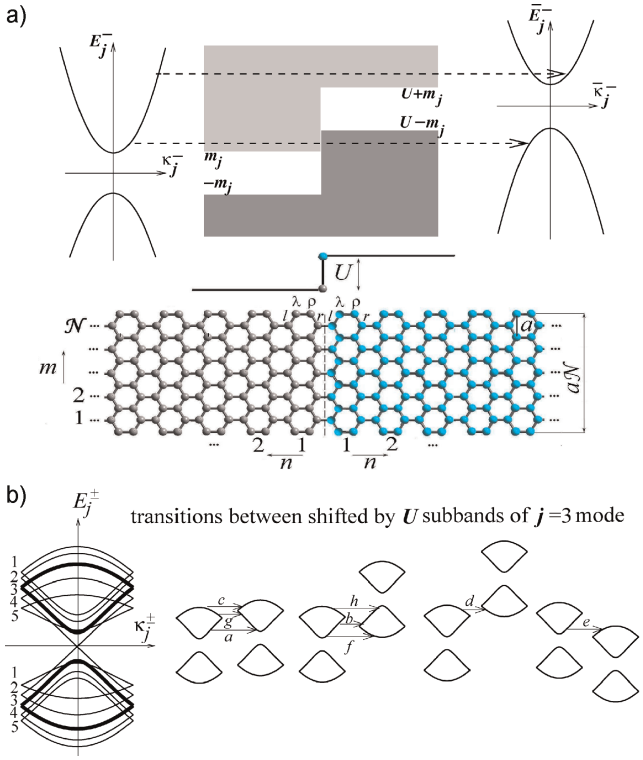

Figure 1 (online color at: www.pss-b.com) (a) Energy diagram of through-step transmission in armchair graphene ribbon (aGR) sketched in gray ($U=0$) and green ($U\neq 0$) but ideal otherwise. It coincides with the diagram of Klein tunneling [1, 2], if on both sides of potential step U, energies of exemplified transitions are close to the jth mode band gap, see Eq. (3). Band gap energy $2m_j$ is specified in Eq. (9). (b) Full band spectrum (3) and possible interband transitions at different energies of incident electron ($E>0$) and step potentials U for $\mathcal{N}=5$-wide aGR. Each of j bands, $j=1,2,\ldots,5$, is subdivided into two valence ($-E_j^\pm$) and two conduction ($E_j^\pm$) subbands. Labels indicate transitions involving either the same subbands, e.g., a corresponds to $E_j^- \to \overline{E}_j^- > 0$ and $b-$ to $E_j^- \to \overline{E}_j^- < 0$, or different subbands, e.g., $E_j^- \to \overline{E}_j^+ > 0$ (e) and $E_j^- \to \overline{E}_j^+ < 0$ (f). Transitions are shown for the one of nonzero gap modes $j=3$. The same classification is used in the text for the zero gap mode j^*, here, $j^*=4$.

v_j ($\overline{v}_j$) is the group velocity of incident (transmitted) wave, and the wavefuction coefficient $\psi_{n,l}^{j\mathrm{R}}$ can easily be found from equations:

$$\begin{aligned}\psi_{nr}^{j\mathrm{L}} &= \psi_{nr}^{0}(\kappa_j^\pm) + G_{nr,1r}^{j\mathrm{L}}(E)\psi_{1l}^{j\mathrm{R}},\\ \psi_{nl}^{j\mathrm{R}} &= G_{nl,1l}^{j\mathrm{R}}(\overline{E})\psi_{1r}^{j\mathrm{L}}.\end{aligned} \tag{2}$$

In this calculation scheme, $\psi_{nr}^{0}(\kappa_j^\pm) = A_j^\pm\, \mathrm{e}^{\mathrm{i}\kappa_j^\pm n} + \text{c.c.}$, $|A_j^\pm|^2 = 1$, represents the solution of the scattering problem for the semi-infinite aGR terminated by r (or l) sites. The dispersion relations $E = E_j^\pm(\kappa_j^\pm)$ and $\overline{E}_j^\pm(\kappa_j^\pm) = E - U$ with the wave vectors of incident and transmitted waves ($\kappa_j^\pm$ and $\overline{\kappa}_j^\pm$) in units of a^{-1}, are given by Ref. [10]:

$$\begin{aligned}\left[E_j^\pm(\kappa_j^\pm)\right]^2 &= \left(1\pm\alpha_j\right)^2 \mp 4\alpha_j\, \sin^2(\kappa_j^\pm/4),\\ 0 \le \kappa_j^\pm &\le \pi,\end{aligned} \tag{3}$$

where $\alpha_j \equiv 2\cos(\xi_j/2)$, and the absolute value of hopping integral t is used as an energy unit. Notation:

$$G_{n,\alpha;1,r}^{j\mathrm{L}} \equiv \sum_{m,m'} \sin(m\xi_j)\sin(m'\xi_j) G_{m,n,\alpha;m',1,r}^{\mathrm{L}}$$

refers to the (multiplied by t) Green's function of semi-infinite aGR terminated by the r or l sites [11]:

$$G_{n,r;1,r}^{j\mathrm{L}}(E) = G_{n,l;1,l}^{j\mathrm{R}}(E) = \frac{g_{ll}^j\, \mathrm{e}^{\mathrm{i}\kappa_j^\pm(n-1)}}{1 - g_{lr}^j\, \mathrm{e}^{\mathrm{i}\kappa_j^\pm}}, \tag{4}$$

$$g_{ll}^j = \frac{E\left(E^2 - 1 - \alpha_j^2\right)}{\left(E^2 - \alpha_j^2\right)^2 - E^2}, \qquad g_{lr}^j = \frac{\alpha_j^2}{\left(E^2 - \alpha_j^2\right)^2 - E^2}. \tag{5}$$

The use of these definitions in Eqs. (1) and (2) yields:

$$T_j = \frac{4\,\mathrm{Im}\, G_{1,r;1,r}^{j\mathrm{L}}(E)\,\mathrm{Im}\, G_{1,l;1,l}^{j\mathrm{R}}(\overline{E})}{\left|1 - G_{1,r;1,r}^{j\mathrm{L}}(E) G_{1,l;1,l}^{j\mathrm{R}}(\overline{E})\right|^2}. \tag{6}$$

Formally, this is the transmission coefficient of a contact via a single hop t between two leads described by Green's functions $G^{j\mathrm{L}}$ and $G^{j\mathrm{R}}$ [9]. In the particular case $\mathcal{N}=j=1$, Eq. (4) represents the Green's function of semi-infinite polyparaphenylene chain M-M-..., M = C_6H_4.

For the purposes of further discussion, Eq. (6) can be transformed as follows:

$$T_j = \begin{cases} \dfrac{4\alpha_j^2\, \sin(\kappa_j^\pm/2)\sin(\overline{\kappa}_j^\pm/2)}{\left|4\alpha_j^2\, \sin^2[(\kappa_j^\pm + (\pm)\overline{\kappa}_j^\pm)/4] - U^2\right|}, & E_j^\pm \to \overline{E}_j^\pm,\\ \dfrac{4\alpha_j^2\, \sin(\kappa_j^\pm/2)\sin(\overline{\kappa}_j^\mp/2)}{\left|4\alpha_j^2\, \cos^2[(\kappa_j^\pm + (\mp)\overline{\kappa}_j^\mp)/4] - U^2\right|}, & E_j^\pm \to \overline{E}_j^\mp, \end{cases} \tag{7}$$

where the upper (lower) sign in ($\pm$) and ($\mp$) refers to $\overline{E} > 0$ ($\overline{E} < 0$). This is equivalent to the Pauli's sign rule noted in Klein's paper [1]. It provides positiveness of group velocities of incident and transmitted waves. In the Green's function language, this is equivalent to the same sign of $\mathrm{Im}\, G_{1,r;1,r}^{j\mathrm{L}}(E)$ and $\mathrm{Im}\, G_{1,r;1,r}^{j\mathrm{L}}(\overline{E})$ at any value of step potential. To pay attention, notation of these signs have a totally different meaning as compared to $\pm$ labeling of dispersion relations $E_j^\pm(\kappa_j^\pm)$ and $\overline{E}_j^\pm(\overline{\kappa}_j^\pm)$ that comes from Eq. (3). In Eq. (7), the energy of incident wave E is assumed positive. From the band spectrum symmetry, $T_j(E>0, U) = T_j(E<0, -U)$.

The first line in Eq. (7) defines the transmission coefficient from "minus" to "minus" and from "plus" to "plus" subband, i.e., it refers to transitions between bands having the same dispersion. In Fig. 1b, these transitions are labeled as $a-d$. The corresponding expressions of T_j represent a detailed form of the result obtained by the mode-matching technique [12]. The

second line in Eq. (7), which defines the transmission coefficient from − to + and from + to − subband ($e-h$ labels in Fig. 1b), gives an essentially different expression of T_j.

Thus, for each of interband transitions illustrated in Fig. 1b, the transmission coefficient has a specific expression in terms of wave vectors of respective subbands, the mode parameter α_j, and potential U. The tunneling energy enters implicitly via $E = E_j^{\pm}(\kappa_j^{\pm})$.

2.1 Long-wave limit Equation (7) is valid for any value of $\mathcal{N}$ and U, and (with small modifications [13]) it can be used to examine the through-step transmission in zigzag carbon tubes of arbitrary diameter. As mentioned, the long wave limit is interesting for establishing the relationship between the tight-binding and Klein descriptions of transitions $E_j^- \to \overline{E}_j^- > 0$ (a) and $E_j^- \to \overline{E}_j^- < 0$ (b).

The fulfillment of conditions $|E - |\alpha_j - 1|| \ll 1$ and $|U| \ll 1$ restricts consideration to small wave vectors, $\kappa_j^-, \overline{\kappa}_j^- \ll 1$, when the dependence $E_j^-(\kappa_j^-)$ becomes similar to the energy–impulse relation of massless ($j = j^*$) or massive ($j \neq j^*$) Dirac fermions. Then, the upper line of Eq. (7) takes the form:

$$
\begin{aligned}
T_{j\neq j^*} &= \frac{2\alpha_j \kappa_j^- \overline{\kappa}_j^-}{\left|\mathrm{sign}(\overline{E}_j^-)\kappa_j^- \overline{\kappa}_j^- + 4\alpha_j^{-1} E_j^- \overline{E}_j^- + Q_j\right|}, \\
Q_j &= \frac{\alpha_j - 1}{2}[\kappa_j^- + \mathrm{sign}(\overline{E}_j^-)\overline{\kappa}_j^-]^2 - 4\frac{(\alpha_j - 1)^2}{\alpha_j}, \\
T_{j^*} &= 1 - \frac{1}{64}[\kappa_{j^*}^- - \mathrm{sign}(\overline{E}_{j^*}^-)\overline{\kappa}_{j^*}^-]^2.
\end{aligned}
\tag{8}
$$

These equations (which are still valid for aGRs of arbitrary width $\mathcal{N}$) are noticeably distinct from Klein's formula showing that formal similarity of energy–impulse relations is not the only condition of relativistic-like behavior of charge carriers in aGR.

For wide ribbons and low energies satisfying $E \ll 1$, the aGR spectrum reads [13]:

$$
\begin{aligned}
E_\nu^-(\kappa_\nu^-) &= \sqrt{m_\nu^2 + (\kappa_\nu^-/2)^2}, \quad \nu = j - \widetilde{j} = 0, \pm 1, ..., \\
m_\nu &= \begin{cases} \dfrac{\sqrt{3}}{2}\dfrac{\pi|\nu|}{\mathcal{N}}\left(1 + \dfrac{\pi\nu}{4\sqrt{3}\mathcal{N}}\right), & \widetilde{j} = j^*, \\ \dfrac{\sqrt{3}}{2}\dfrac{\pi|\nu - (+)1/3|}{\mathcal{N}}, & \widetilde{j} = j_<^*(j_>^*), \end{cases}
\end{aligned}
\tag{9}
$$

where $|\nu| \ll \mathcal{N}$, and $\widetilde{j}$ denotes the lowest-energy band which has zero gap, when $j^* = 2(\mathcal{N}+1)/3$ is an integer, and it has nonzero gap, when either $j_<^* = (2\mathcal{N}+1)/3$ or $j_>^* = (2\mathcal{N}+3)/3$ is an integer. If and only if Eq. (9) works well, deviations of α_j from unity give higher-order corrections to Eq. (8) and can be disregarded. This makes the expression of $T_{j\neq j^*}$ totally equivalent to Klein's formula:

$$
T_\nu = \frac{4K_\nu}{(1+K_\nu)^2}, \quad K_\nu = \sqrt{\frac{(E+m_\nu)(\overline{E}-m_\nu)}{(E-m_\nu)(\overline{E}+m_\nu)}}, \tag{10}
$$

which form is borrowed from [2] because it is convenient for comparison [14].

It is seen that in this approximation, $T_{j^*} = T_{\nu=0} = 1$, but for all other modes $T_\nu < 1$ at any nonzero potential. However, the tight-binding model predicts an essentially different behavior of mode transmission, particularly, for narrow aGRs. This is illustrated in Fig. 2 and will be discussed next.

2.2 Transmission without backscattering, $T_j = 1$ The consistency of each expression that follows from Eq. (7) with the unit mode transmission, $T_j = 1$, at $U \neq 0$, has been examined in detail. This analysis leads to the conclusion that, except j^*-mode transmission, the absence of backscattering is realized for certain transitions at certain magnitude of step potential $U = U_j^r$ related to the energy of transmitted particle as:

$$
U_{j\neq j^*}^r = E + \frac{\alpha_j^2 - 1}{E}. \tag{11}
$$

Some immediate conclusions from this equation regarding the magnitude of mode parameter ($0 < \alpha_j < 2$) and the position of unit transmission $T_j(U_j^r) = 1$ with respect to the region of zero transmission, $T_j(U) = 0$ at $E - |1 - \alpha_j| \leq U \leq E + |1 - \alpha_j|$, i.e., a deep in the dependence $T_j(U)$, are noteworthy.

For all modes with $\alpha_j > 1$ (for brevity, $j_<$ modes), the unit transmission is above the deep, $U > E + |1 - \alpha_j|$ (to the right in the picture), and can involve transitions $E_j^- \to \overline{E}_j^{\pm} < 0$ (b and f) or $E_j^+ \to \overline{E}_j^- < 0$ (h). In contrast, the condition $\alpha_j < 1$ places the unit transmission of $j_>$ modes bellow the deep, and associated transitions are only $E_j^- \to \overline{E}_j^{\pm} > 0$ (a and e) or $E_j^+ \to \overline{E}_j^- > 0$ (g). As a consequence, for modes divided by this criterion (for example, it concerns j^*+1 and j^*+1 as well as $j_<^*$ and $j_>^*$ modes) dependencies $T_{j_<}(U)$ and $T_{j_>}(U)$ may have a strikingly different appearance as illustrated in Fig. 2.

These results suggest that in an appropriately designed experiment, semiconducting aGRs having $\widetilde{j} = j_<^*$ can be distinguished from those, where $\widetilde{j} = j_>^*$. To achieve this, at least two requirements should be met. First, the possibility to control the regimes of single- and two-mode current. Second, the access to nanowide ribbons because tunneling energies are restricted to small values by experimental conditions. At $E \ll 1$, the increase of ribbon width wipes off the difference between transmission of low-energy modes $j_<$ and $j_>$. Therefore, manifestation of our predictions in measurements of source-to-drain current under varied gate voltage (playing the role of step potential) can be expected only for narrow ribbons with $\mathcal{N} \sim 20$ (about 5 nm) or less.

The substantially different behavior of $T_{j_<}(U)$ and $T_{j_>}(U)$ is the direct consequence of that the $j_<$ mode unit

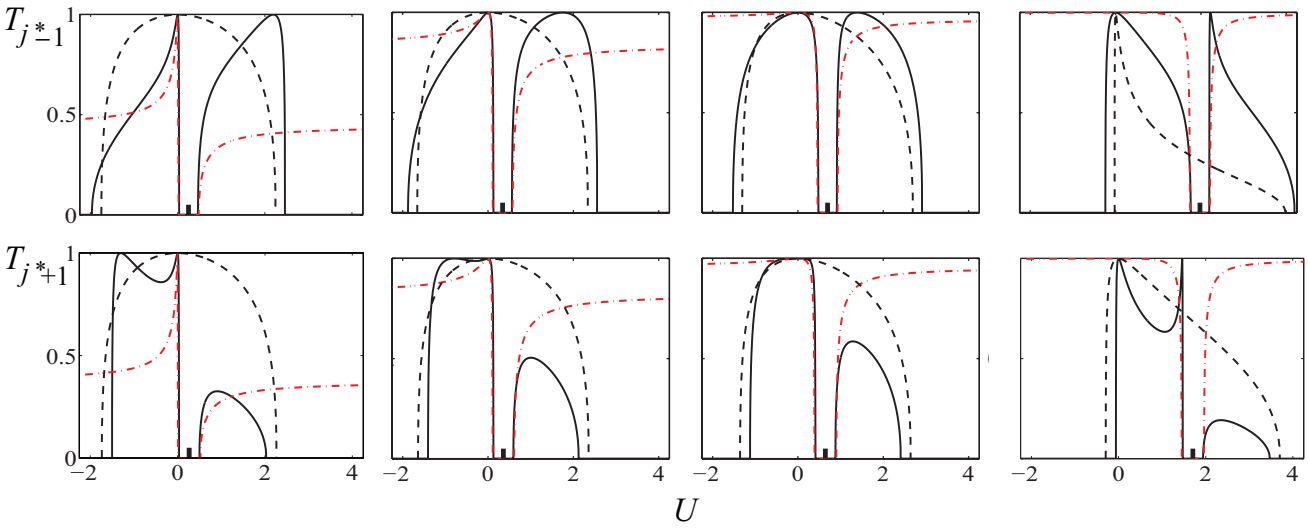

Figure 2 (online color at: www.pss-b.com) Through-step transmission coefficient $T_j(U)$ of $\mathcal{N} = 11$ – wide armchair graphene ribbon. Calculations according to Eq. (7) are represented by black solid (T_7, T_9) and dashed ($T_{j^*=8}$) lines. Approximation (10) for T_7 and T_9 is shown by red dashed-dotted lines. Thick vertical bars on U axes indicate tunneling energies (from left to right): $E \approx |\alpha_j - 1|$ (near the bottom of subband E_j^-), $|\alpha_j - 1| < E < \sqrt{|\alpha_j^2 - 1|}$, $E = \sqrt{|\alpha_j^2 - 1|}$, and $E \approx \alpha_j + 1$ (near the top of subband E_j^+).

transmission must always be to the right of deeps in Fig. 2, whereas for $j_>$ modes, it is always placed to the left. For the same reason, the transmission spectrum of polyparaphenylene (not shown but hardly distinguishable from $T_{j^*-1=7}$ in Fig. 2), where the mode parameter takes the value of $\alpha_1 = \sqrt{2} > 1$, is very similar to $T_{j_<}(U)$ of narrow aGRs. Thus, the visial row T_{j^*-1} in Fig. 2 appears to be intimately related to electron transmitting properties of polyparaphenylene. The origin of distinctive shape of $T_{j_>}(U)$ has another nature. It can rather be thought as a peculiar effect or manifestation of edge states at graphene sheet zigzag edges [15]. Indeed, if we cut an infinite aGR across l–r bonds, the edge states appear in the respective semi-infinite parts, but only for $j_>$ modes [13]. Therefore, the corresponding Green's functions in Eq. (6) do not have or have a pole at zero energy depending on whether $j < j^*$ or $j > j^*$ ($j \le j^*_<$ or $j \ge j^*_<$). This explains the difference between $T_{j_<}(U)$ and $T_{j_>}(U)$ although the surface states themselves do not contribute to the transmission because of their localization at zigzag edges.

In conclusion, it is shown that in aGRs, the through-step transmission coefficient can be explicitly related to all associated transitions between subbands of the given mode. As an approximation of exact expressions obtained here, Klein's tunneling formula is re-derived and its range of applicability is demonstrated. Also, the step potential, at which the mode transmission occurs with unit probability, is obtained in the form of a function of tunneling energy and mode parameter. Physics and experimental implications of this result have been briefly discussed.

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