Lattice propagation determined oblique perfect transmission in atomically-sharp graphene p-n junctions

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Due to the simplicity of lattice and electronic structures, graphene has been an ideal platform to explore the transport of Dirac fermions. However, the influence of a such simple lattice on the exotic transport phenomena has not been well understood yet. Here, based on the lattice model, we solve analytically the condition for the perfect transmission of electrons across atomically-sharp graphene p-n junctions. Unexpectedly, Klein tunneling does not exist even for the Dirac fermions in the linear energy regime, whereas perfect transmission at oblique incidence always persists. Strikingly, the critical incident angle \( \theta_{\text{PT}} \) for oblique perfect transmission has an analytical expression \( \theta_{\text{PT}} \approx (3\pi/2)(a_0/\lambda_F) \), in which \( a_0 \) is the carbon-carbon bond length and \( \lambda_F \) is the Fermi wavelength of electrons in the right transmission region. i) The lattice origin of \( \theta_{\text{PT}} \approx a_0 \) reveals a hitherto unidentified lattice propagation effect. ii) \( \theta_{\text{PT}} \approx 1/\lambda_F \approx \varepsilon_R \) with \( \varepsilon_R \) the doping level of the transmission region favors the superior tunability comparing to the independence on the doping level of Klein tunneling. This study shows the importance of graphene as a model material to in-depth explore the Dirac physics and highlights the atomically-scale study of electronic transport in Dirac materials.

I. INTRODUCTION

Graphene is the representative system of various Dirac and/or two-dimensional materials with simple electronic and lattice structures, in which the electronic transport has the importance in fundamental physics and realistic applications. On one hand, the high mobility of graphene favors superior ballistic transport, which is very sensitive to the atomically-scale scattering potential induced by the single vacancy or impurity, edge geometries, a line defect, and so on. On the other hand, the long ballistic length makes graphene be promising to construct the devices used in electron optics. The basic component of various devices in electron optics and other fields is the p-n junction structure. The graphene p-n junction has brought many novel physical properties, e.g., Klein tunneling, Veselago focusing, wave guiding, and quantum Goos-Hänchen effect. Klein tunneling is an outstanding example of exotic transport in graphene. Usually, the electronic structure (i.e., the band geometry at the Fermi level), is deemed as the dominant factor in determining the Klein tunneling (and other transport phenomena). However, the influence of the simple lattice structure of graphene on the Klein tunneling has not been well understood yet.

For a graphene p-n junction (see Fig. 1), there are four length scales including the Fermi wavelengths of carriers \( \lambda_{L,R} \) in left and right regions, the junction width \( w \) and the carbon-carbon bond length \( a_0 \). Comparing to these length scales, one can divide graphene junctions into three typical classes: (i) a nominal sharp junction with \( a_0 \ll w \ll \min(\lambda_L, \lambda_R) \), (ii) a smooth junction with \( a_0 \ll \min(\lambda_L, \lambda_R) \ll w \) and (iii) an atomically-sharp junction with \( a_0 \leq w \ll \min(\lambda_L, \lambda_R) \). For graphene, the seminal paper on Klein tunneling considers the class (i) while another important paper studies the class (ii) for the first time. Ref. [21] also points out that the whole physical picture of class (i) and (ii) may be changed dramatically in the class (iii), and the continuum model is not applicable to class (iii). As a result, people have to use the lattice model to consider class (iii). However, limited to the existing cognition on Klein tunneling, people mainly consider the electron transmission at normal incidence for the symmetrical p-n junction and perform the rough generalization of the conclusions of classes (i) and (ii) to class (iii), this leads to the concealing of new physics in class (iii) or the atomically-sharp junction.

In this study, boosted by the experimental fabrication of the atomically-sharp p-n junction, we revisit the Klein tunneling by using the lattice model in an analytical manner. Unexpectedly, Klein tunneling does not exist even for Dirac fermions, whereas perfect transmission at oblique incidence occurs. And the critical incident angle for oblique perfect transmission is dominated by the lattice propagation effect unique to the lattice model over the band geometry, and can not be described by any continuum model. This study implies the importance of lattice propagation at the atomic scale in understanding the novel transport properties of Dirac materials.

II. THEORETICAL FORMALISM

A. Model

Fig. 1 shows a sharp graphene junction with two separating left and right regions in different colors. Fig. 1 is the ultimate form of the atomically-sharp junction in experiment, and has been considered numerically but not been treated analytical yet. The junction interface of Fig. 1 is chosen along the zigzag direction, then the intervalley scattering which may affect the Klein tunneling does not occur. The lattice Hamiltonian of the junction is the sum of the lattice Hamiltonian for uniform graphene, and the on-site junction potential which adopts the constant \( -V_0 \) for all the carbon sites in the left (right) region (see the inset of Fig. 1). The aligned Fermi level \( E_F \) determines the doping level in left and right regions as \( \varepsilon_L \equiv E_F + V_0 \) (\( \varepsilon_R \equiv E_F - V_0 \)) with a positive (negative) doping level corresponding to electron or N (hole or P) doping.
FIG. 1. Schematic atomically-sharp graphene junction in the Cartesian coordinate system with basis vectors \((e_x, e_y)\). In the blue dotted rectangle, two lattice sites \(A\) and \(B\) lying at two sides of junction interface are used for the matching condition of the scattering states across the junction. The inset sketches the Dirac points shifted by the junction potentials \(-V_0\) and \(V_0\) in the left region and the right region. In addition, one lattice unit vector is introduced (i.e., \(\tau = -3/2e_x + \sqrt{3}/2e_y\)), along which the lattice propagation phase accumulates.\(^{25}\)

Previously, we have developed an analytical mode-matching technique in the lattice model\(^{24}\) to describe electron transport across various graphene junctions. The key of the developed technique is the matching of the scattering states at two lattice sites (see Ref. 24 for technique details), which is very different from the matching at one single spatial position but for two atoms in the continuum model\(^{14}\). Finally, the mode-matching condition can be collected as\(^{24}\):

\[
|u_i⟩ + c_r|u_t⟩ = c_t e^{i\kappa \tau} |u_t⟩. \tag{1}
\]

Here, \(\alpha = (i, r, t)\) denotes the incident, reflection, and transmission traveling eigenstates, \(\kappa = (k_x, k_y)\) is the momentum of each state, \(c_{ir}\) are the reflection and transmission coefficients, and \(\tau = -3/2e_x - \sqrt{3}/2e_y\) is one lattice unit vector.

Most importantly, \(|u_t⟩ = \{1, e^{i(\phi - \kappa \cdot \tau)}\}^T\) is a renormalized spinor state\(^{24}\) and its up and down components represent the wave amplitudes on the lattice sites \(A\) and \(B\) lying at two sides of junction interface, e.g., the sites in the blue dotted rectangle in Fig. 1. The down component of \(|u_t⟩\) is renormalized by the lattice propagation determined phase \(e^{i\kappa \cdot \tau}\) beyond the usual phases \(e^{i\phi}\) contributed by the band geometry. The band geometry introduces the phases\(^{24}\):

\[
e^{i\phi_i} \equiv \frac{f^+(\kappa)}{|f(\kappa)|} = \frac{f^+(\kappa)}{\varepsilon_L}, \tag{2a}
\]
\[
e^{i\phi_r} \equiv \frac{f^-(\kappa)}{|f(\kappa)|} = \frac{f^-(\kappa)}{\varepsilon_L}, \tag{2b}
\]
\[
e^{i\phi_t} \equiv \frac{f^+(\kappa)}{|f(\kappa)|} = \frac{f^+(\kappa)}{\varepsilon_R}, \tag{2c}
\]

through the energy spectrum

\[
\varepsilon_L = |f(\kappa)| = |f(\kappa)|, \tag{3a}
\]
\[
\varepsilon_R = |f(\kappa)|, \tag{3b}
\]

where \(f(\kappa) = -(1 + e^{i\sqrt{3}k_y} + e^{-i\sqrt{3}k_y})\). The lattice propagation phase \(e^{i\kappa \cdot \tau}\) accumulates over one unit cell and couples two sites belonging to different regions of the junction, this effect is unique to the lattice model and has not been identified yet in graphene junctions. Noting here, we use the carbon-carbon bond length \(a_0 = 0.142\) nm as the unit of length and the nearest-neighbor hopping energy \(t_0 = 2.7\) eV as the unit of energy.\(^{24}\)

**B. Critical angle for perfect transmission**

Due to the conservation of the generalized pseudospin in the lattice model, the perfect transmission always persists and the condition of perfect transmission for electrons across the atomically-sharp junction is\(^{24}\):

\[
e^{i(\phi_r - \kappa \cdot \tau)} = e^{i(\phi_t - \kappa \cdot \tau)}. \tag{4}
\]

Eq. (4) is the necessary condition for perfect transmission.\(^{24}\) In this study, we use Eq. (4) as the starting point to analytically determine the critical momentum \(q_{PT}\) and/or angle \(\theta_{PT}\) for perfect transmission. The transmission probability \(T(k_y)\) to be an even function of \(k_y\) due to the mirror symmetry of the junction about the \(x\) axis (see Fig. 1), so we can limit our derivations to one valley, say \(K = (0, \pm \sqrt{3}/2)\). Introducing the reduced momentum \(q_y = k_y - K\), Eq. (4) can be rewritten as

\[
e^{i\phi} = \frac{e^{i\phi_i}}{e^{i\phi_r}}, \tag{5}
\]

The left (right) hand side originates from the band geometry (lattice propagation) phases of the incident and transmission eigenstates. And \(v_f = 3/2\) is the Fermi velocity in the continuum limit.\(^{24}\) Using Eq. (2) and \(k_y = q_y + K\), we obtain

\[
\frac{e^{i\phi_i}}{e^{i\phi_r}} = \frac{\varepsilon_L}{\varepsilon_R} \cdot \frac{2 \cos(\sqrt{3}q_y)}{\cos(\sqrt{3}q_y)}, \tag{6}
\]

where \(\tilde{q}_y = \pi/3 + \sqrt{3}q_y/2\). Substituting into Eq. (5) and taking the real part gives

\[
\frac{\varepsilon_L}{\varepsilon_R} = \frac{2 \cos(v_f q_{xl})}{\cos(\sqrt{3}q_y)}, \tag{7}
\]

The condition that \(q_y\) and \(q_x\) lie on the Fermi level \(\{\text{i.e., Eq. (4)}\}\) allows us to express \(q_{xl}\) and \(q_{yr}\) in terms of \(\tilde{q}_y\), so Eq. (7) becomes a closed equation for \(\tilde{q}_y\), from which we obtain

\[
q_{PT} = \frac{2}{\sqrt{3}} \left( \frac{\cos^{-1} \sqrt{1 - \varepsilon_L \varepsilon_R} - \pi}{3} \right), \tag{8}
\]

and hence

\[
\cos(v_f q_{xl}) = \frac{1 - \varepsilon_L \varepsilon_R}{\sqrt{1 - \varepsilon_L \varepsilon_R}}, \tag{9a}
\]
\[
\cos(v_f q_{yr}) = \frac{1 - \varepsilon_L \varepsilon_R}{\sqrt{1 - \varepsilon_L \varepsilon_R}}. \tag{9b}
\]

where we have used the fact that \(q_i \in [-2\pi/(3\sqrt{3}), \pi/(3\sqrt{3})]\) and \(q_x \in [-\pi/3, \pi/3]\) in the \(K\) valley,\(^{24}\) so that \(\tilde{q}_y \in [0, \pi/2]\).
Equations (8) and (9) are valid as long as the doping is below the Van Hove singularity ($|\varepsilon_L|, |\varepsilon_R| < 1$) of electronic structure of graphene. These equations together with the requirement that the incident wave $q_i$ and the transmission wave $q_f$ must have a positive group velocity along the $+x$ axis uniquely determine $q_i$ and $q_f$. Finally, we specialize to low doping $|\varepsilon_{L,R}| \ll 1$, in this case, Eq. (8) gives

$$q_{y,PT} \approx \frac{\varepsilon_L \varepsilon_R}{3},$$

and hence

$$\sin \theta_{PT} \approx \frac{\varepsilon_R}{2}.$$

Here, we have used $q_{y,PT} = (\varepsilon_L/V_F) \sin \theta_{PT}$, then we obtain

$$\theta_{PT} \approx \frac{\varepsilon_R}{2} = \frac{E_F - V_0}{2} = \frac{3\pi a_0}{2 \lambda_R}.$$  

In the Equation (12), we recover the units to show the dimensionless properties of $\theta_{PT}$. Equation (12) is the main result of this study, and has three implications: (i) $\theta_{PT} \approx 0$ shows the oblique perfect transmission in contrast to Klein tunneling at normal incidence ($\theta_{PT} = 0$)\(^{12,14}\), (ii) $\theta_{PT} \approx (3\pi/2)(a_0/\lambda_R)$ which clearly shows the lattice nature of the oblique perfect transmission. Usually, $\theta_{PT}$ should be small since $a_0 \ll \lambda_R$. However, the unique lattice structure of graphene makes $\theta_{PT}$ very appreciable due to the large prefactor $3\pi/2$. (iii) $\theta_{PT}$ only depends on the doping level $\varepsilon_R$ of the right or transmission region and increases linearly with $\varepsilon_R$, this means the superior tunability comparing the independence on the doping level of Klein tunneling. Next we analyze and distinguish the physical mechanisms underlying the oblique perfect transmission by comparing the contributions of lattice propagation and band geometry.

C. Lattice propagation vs band geometry

Based on the Eq. (5), the left hand side is the spinor phases incorporating the band geometry while the right hand side is the lattice propagation phases. By using the lattice model, we can properly consider the band geometry, e.g., the obvious trigonal warping of energy band with increasing the doping level\(^{12}\). However, the lattice propagation effect is not included in any continuum model, so it is a unique feature of the lattice model. To identify the importance of lattice propagation phases, we derive the critical momentum and angle in the absence of lattice propagation effect, i.e., we set $e^{i\phi_{q_{x,0}}} / e^{i\phi_{q_{x,0} \perp}} = 1$ and calculate the spinor phases $e^{i\phi_{e}}$ and $e^{i\phi_{\perp}}$ exactly according to Eq. (3). The results for $e^{i\phi_{e}}$, $e^{i\phi_{\perp}}$ are given by Eq. (6), thus the perfect transmission condition Eq. (5) reduces to

$$\frac{\varepsilon_R 2 \cos q'_{x,PT} - \cos (\nu_F q'_{x,PT})}{\varepsilon_L 2 \cos q'_x - \cos (\nu_F q'_x)} = 1.$$  

III. NUMERICAL RESULTS AND DISCUSSIONS

Fig. 2 shows the dependence behaviors of critical angle $\theta_{PT}$ for perfect transmission on the junction potential $V_0$ and

![Graph showing the dependence of critical angle $\theta_{PT}$ on junction potential $V_0$.]
the Fermi level $E_F$, in which we also present the exact results calculated by using the lattice Green’s function.\textsuperscript{22,28} Surprisingly, over a wide doping level and even beyond the linear Dirac regime (e.g., $\max|\epsilon_L - \epsilon_R| \approx 0.5$), the exact results agree well with the simple analytical expressions in Eq. (12). The consistence confirms the usefulness of Eq. (12) to describe the parameter dependence of $\theta_{PT}$, and highlights the linear increase of $\theta_{PT}$ with the doping level $\epsilon_R$ of the transmission states when we consider incident states from left region of the $p$-$n$ junction.

Besides the well-known normal Klein tunneling, the oblique Klein tunneling can be induced by the magnetic barrier\textsuperscript{26} and by the unusual band geometries such as the anisotropic, tilted\textsuperscript{27,28} and the oblique Klein tunneling\textsuperscript{29,30} due to unusual band geometries which both have no dependence on the doping level, the discovered oblique perfect transmission can be tuned electrically since the gate doping is widely used for graphene and other two-dimensional materials. The electrically-tunable critical angle of oblique perfect transmission should be beneficial to its experimental observation (e.g., by applying the dual-probe scanning tunneling microscopy) on the atomically-sharp graphene $p$-$n$ junction\textsuperscript{30,31}, and potential applications. Finally, we emphasize that the lattice propagation effect should have profound implication for the other exotic transport phenomena such as Veselago focusing, quantum Goos-Hänchen effect and wave guiding in graphene and other Dirac materials.

In this study, for brevity, we focus the electrons of $K$ valley across the $p$-$n$ junction with $\epsilon_L > 0$ and $\epsilon_R < 0$. Firstly, the generalization to the electrons in the other valley across other junctions is straightforward since our derivations in Sec. II are applicable to various junctions, such as N-N junction ($\epsilon_L, \epsilon_R > 0$), P-P junction ($\epsilon_L, \epsilon_R < 0$), and P-N junction ($\epsilon_L \epsilon_R < 0$). Secondly, two inequivalent valleys of graphene have the mirror symmetry about the $x$-axis in the junction with the zigzag interface, so the transmission of electrons in two valleys across the junctions are related to each other and the intervalley scattering requiring the conservation of momentum $k_y$ does not exist\textsuperscript{32}. Thirdly, we hope the lattice propagation effect can be verified experimentally in near future, and very relevant experiential feasibility has been presented in our previous work\textsuperscript{24}. Finally, it is a challenging task to analytically reveal the evolution mechanism of oblique perfect transmission in the atomically-sharp junction to the normal Klein tunneling in the nominal sharp junction\textsuperscript{26} and the smooth junction\textsuperscript{22}.

IV. CONCLUSIONS

Klein tunneling is one well-known relativistic phenomena in graphene, it is interesting to explore the possible influence of electron propagation at the atomic scale on it. To this aim, for atomically-sharp graphene $p$-$n$ junctions, we solve analytically the condition for the perfect transmission derived from the lattice model. Klein tunneling is found to disappear even in the linear energy regime, while perfect transmission at oblique incidence always persists. For the oblique perfect transmission, we also obtain an explicit analytical expression of the critical incident angle $\theta_{PT} \approx (3\pi/2)\epsilon_0/\lambda_R$, which clearly shows its lattice nature and tunability. As a result, comparing to the band geometry effect\textsuperscript{29–32}, a hitherto lattice propagation effect unique to the lattice model is identified. This study is relevant to the deep understanding of the electronic transport at atomic scale in graphene and other Dirac materials.

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