Suppressing Klein tunneling in graphene using a one-dimensional array of localized scatterers

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Graphene’s unique physical and chemical properties make it an attractive platform for use in micro- and nanoelectronic devices. However, electrostatically controlling the flow of electrons in graphene can be challenging as a result of Klein tunneling, where electrons normally incident to a one-dimensional potential barrier of height $V$ are perfectly transmitted even as $V \to \infty$. In this study, theoretical and numerical calculations predict that the transmission probability for an electron wave normally incident to a one-dimensional array of localized scatterers can be significantly less than unity when the electron wavelength is smaller than the spacing between scatterers. In effect, placing periodic openings throughout a potential barrier can, somewhat counterintuitively, decrease transmission in graphene. Our results suggest that electrostatic potentials with spatial variations on the order of the electron wavelength can suppress Klein tunneling and could find applications in developing graphene electronic devices.

Since graphene’s initial discovery, much research has been undertaken into studying graphene’s unique physical and chemical properties, which are a consequence of its two-dimensional structure. Graphene consists of carbon atoms arranged in a honeycomb lattice made up of two trigonal sublattices that each contribute a carbon atom to the unit cell, thereby imparting a pseudospin character to the electrons in graphene. From tight-binding calculations, the quasiparticle spectrum of graphene is linearly proportional to the magnitude of the wave vector, $|\mathbf{k}|$, when expanded about two distinct wave vectors, $\pm \mathbf{K}$, with $b = 1.42 \text{ Å}$ being the C-C bond length. The wave vectors $\pm \mathbf{K}$ are referred to as Dirac points due to the similarity of the electronic spectrum in graphene to that of a massless two-dimensional Dirac fermion. A consequence of the linear dispersion and the pseudospin nature of electron waves in graphene is Klein tunneling, where massless Dirac fermions normally incident to a potential step barrier are not reflected even when the potential barrier height becomes infinite (Figure 1(A)). Klein tunneling makes it difficult to stop the flow or transmission of electrons electrostatically, which poses a significant challenge for incorporating graphene into new electronic devices.

One proposed method for controlling and modifying the electronic properties in graphene has been to use superlattice potentials, $V(x,y)$. In this case, graphene’s effective Hamiltonian, when expanded about the $\pm \mathbf{K}$ Dirac points, is given by:

$$\hat{H}_{\pm \mathbf{K}} = \pm \hbar v_F (\hat{\sigma}_X \hat{p}_X + \hat{\sigma}_Y \hat{p}_Y) + V(x,y)$$  \hspace{1cm} (1)$$

where $\hat{\sigma}_X$ and $\hat{\sigma}_Y$ are pauli spin matrices, $\hat{p}_X$ and $\hat{p}_Y$ are momentum operators, and $\hbar v_F = 1.0558 \times 10^{-26}$ J·m. In writing Eq. (1), the spatial variations of $V(x,y)$ are assumed to be on length scales much greater than the C-C bond length. Such superlattice potentials can, in principle, be patterned on graphene using either localized chemical modifications or by locally manipulating the voltages of metallic islands or electrodes placed on top of graphene. Previous theoretical work has mainly focused on using periodic potentials along a single dimension, e.g., a periodic array of square potential barriers like the one shown in Fig. 1(A). For such a Kronig-Penney potential, there is no suppression of Klein tunneling for electrons at normal incidence. Other types of superlattice potentials, such as the muffin-tin superlattice potential, which consists of a two-dimensional array of cylindrically symmetric step potentials, have been theoretically shown to generate electron localization and significantly alter graphene’s dispersion relationship although the transport properties through such superlattice potentials have not been examined.
intervalley scattering \( \tilde{k} + \tilde{K} \rightarrow \tilde{K} + \tilde{K} \), \( r_i \) must be greater than the C-C bond length in graphene, i.e., \( r_i > 1.42 \text{ Å} \).

As derived in Supporting Information, the transmitted wave function \( \chi_{\tilde{K}X}^{+} \), \( \psi_{\tilde{K}X}^{+} (\tilde{r}) \), can be written as a sum of Dirac plane wave spinors with wave vectors along the Bragg directions, \( \tilde{k}^{(n)} = k_{Y1}^{(n)} \hat{y} + k_{X1}^{(n)} \hat{x} \) for integer \( n \) where \( k_{Y1}^{(n)} = k_{Y1} + \frac{2mn}{d} \) and \( k_{X1}^{(n)} = k_{X1}^{(n)} \) for \( k_{1} \geq k_{Y1}^{(n)} \). In this case, the transmitted wave function through the one-dimensional array of localized scatterers can be written as a sum over Dirac plane wave spinors propagating along the Bragg directions for \( x \gg d \) as:

\[
\psi_{\tilde{K}X}^{+} (\tilde{r}) = \sum_{n \in \mathcal{N}} T_n e^{i(k_{Y1}^{(n)}y + k_{X1}^{(n)}x)} \sqrt{\frac{k_1}{2V_{r_1}k_{X1}^{(n)}}} \left( 1 + e^{-i\theta_{k_1}} \right)_{\tilde{r}} \pm \tilde{K} \tag{2}
\]

where \( T_n \) is the transmission coefficient for the \( n \)-th Bragg direction or open scattering channel. The sum in Eq. (2) is over all open scattering channels, \( n \in \mathcal{N} = [\mathcal{N}_{\text{min}}, \mathcal{N}_{\text{max}}] \), where \( \mathcal{N}_{\text{min}} = \left\{ -(k_1 + k_{Y1}) d \right\} / \pi \) and \( \mathcal{N}_{\text{max}} = \left\{ (k_1 - k_{Y1}) d \right\} / \pi \), where \( \{ \} \) corresponds to the smallest integer greater than \( z \), and \( \{ \} \) corresponds to the largest integer less than \( z \).

Likewise, the reflected wave function \( x \ll -d \) is given by:

\[
\psi_{\tilde{K}X}^{-} (\tilde{r}) = \sum_{n \in \mathcal{N}} R_n e^{i(k_{Y1}^{(n)}y - k_{X1}^{(n)}x)} \sqrt{\frac{k_1}{2V_{r_1}k_{X1}^{(n)}}} \left( 1 + e^{-i\theta_{k_1}} \right)_{\tilde{r}} \pm \tilde{K} \tag{3}
\]

where \( R_n \) is the reflection coefficient for the \( n \)-th open scattering channel in \( \mathcal{N} \). Due to the unitarity condition, \( \sum_{n \in \mathcal{N}} |R_n|^2 + |T_n|^2 = 1 \). Expressions for \( R_n \) and \( T_n \) are given in Supporting Information.

In Fig. 2, numerical calculations of the total transmission probability, \( T_{\text{tot}} = \sum_{n \in \mathcal{N}} |T_n|^2 \), for \( \theta_{k_1} = 0 \) to a one-dimensional array of localized cylindrically symmetric scatterers of radius \( r_s = 20 \text{ nm} \) as a function of \( \frac{d}{\lambda} \) are shown for the following scattering potentials and lattice spacings: (black) \( V_0 = 0.8 \text{ eV} \) and \( d = 150 \text{ nm} \), (green) \( V_0 = 0.2 \text{ eV} \) and \( d = 150 \text{ nm} \), and (blue) \( V_0 = -0.9683 \text{ eV} \) and \( d = 156.5 \text{ nm} \). For reference, \( T_{\text{tot}} = 1 \) is represented by a red line, which is the exact transmission probability for a wave normally incident to a constant one-dimensional potential barrier\textsuperscript{19} as shown in Fig. 1(A). For \( \lambda \ll d \), \( T_{\text{tot}} = 1 \) for all \( V_0 \) since only the \( n = 0 \) scattering channel is open, i.e., \( \mathcal{N} = \{ 0 \} \).

As a result, the incident electron wave is prohibited from direct backscattering due to time-reversal symmetry leading to \( T_{\text{tot}} = 1 \). This can also be understood by the fact that when \( \lambda \ll d \), the scattering effectively appears as a constant one-dimensional potential barrier [Fig. 1(A)] where \( T_{\text{tot}} = 1 \) for \( \theta_{k_1} = 0 \). However, when \( \lambda \geq 1 \), the incident wave can now backscatter into additional open scattering channels, \( k_{Y1}^{(n)} \) and \( k_{X1}^{(n)} \), for \( n \neq 0 \) in Eq. (3), that do not correspond to direct backscattering, thereby leading to \( T_{\text{tot}} \leq 1 \). Although additional open scattering channels are now available for the incident electron wave to scatter into when \( \lambda \geq 1 \) for \( \theta_{k_1} = 0 \), \( T_{\text{tot}} \) depends on \( V_0 \). For example, \( T_{\text{tot}} \) decreased to 0.6277 at \( \lambda = 1.01 \) for \( V_0 = 0.8 \text{ eV} \) and \( d = 150 \text{ nm} \) [Fig. 2, black curve] and \( T_{\text{tot}} = 0.0134 \) at \( \lambda = 1.1855 \) for \( V_0 = -0.9683 \text{ eV} \) and \( d = 31.3 \text{ nm} \) [Fig. 1, blue curve].

At non-normal incidence, the incident Dirac plane wave can undergo specular reflection and therefore have \( T_{\text{tot}} < 1 \). In
Figure 2 | (A) Scattering of an incident Dirac plane wave spinor of energy \( E = \hbar v k \) \( \geq 0 \), \( \phi_{\text{inc}}(r) = \frac{k_1}{2\pi k_{X1}} e^{ik_1 r} \left( \pm e^{ik_1 r} \right) \), from a one-dimensional array of localized cylindrically symmetric scatterers in graphene. The unit cell for the scattering array consists of a single scatterer with the position of the \( n^{\text{th}} \) scatterer given by \( \vec{r}_n = n \vec{d} \). (B) Transmission probability, \( T_{\text{tot}} \), for a plane wave normally incident \( \theta_{k_1} = 0 \) to either a (red line) one-dimensional potential barrier of width 40 nm \( [T_{\text{tot}} = 1 \text{ for all potentials studied in this work}] \) or a one-dimensional array of localized cylindrically symmetric scatterers of radius \( r_s = 20 \text{ nm} \) with the following scattering potentials and lattice spacings: (blue) \( V_0 = -0.9683 \text{ eV} \) and \( d = 150.5 \text{ nm} \), (green) \( V_0 = 0.2 \text{ eV} \) and \( d = 150 \text{ nm} \), and (black) \( V_0 = 0.8 \text{ eV} \) and \( d = 150 \text{ nm} \). For \( \frac{d}{\lambda} \ll 1 \), the one-dimensional array of scatterers appear as a uniform one-dimensional potential barrier (black and green) or well (blue) and thus \( T_{\text{tot}} = 1 \). When \( \frac{d}{\lambda} \geq 1 \), however, the incident electron wave can be reflected into waves with wave vectors \( -k_{X1} \hat{x} + k_{Z1} \hat{y} \) for \( n \neq 0 \) that do not correspond to direct backscattering. As a result, \( T_{\text{tot}} \leq 1 \) when \( \frac{d}{\lambda} \geq 1 \).

Figure 3, a comparison of \( T_{\text{tot}} \) as a function of \( \frac{d}{\lambda} \) at \( \theta_{k_1} = \frac{1}{2\pi} \), in graphene is shown [Fig. 3, right]. For comparison, the total transmission probability for non-spinor or achiral plane waves found in a regular two-dimensional electron gas (2DEG) with \( \mathcal{H}_{2\text{DEG}} = \frac{\hbar^2}{2m} \nabla^2 + V(x, y) \) is also shown [Fig. 3, left]. The same scattering potentials and lattice spacings used in Figure 2 were also used in the calculations shown in Fig. 3: [Fig. 3(A)] \( V_0 = 0.2 \text{ eV} \) and \( d = 150 \text{ nm} \), [Fig. 3(B)] \( V_0 = 0.8 \text{ eV} \) and \( d = 150 \text{ nm} \), and [Fig. 3(C)] \( V_0 = -0.9683 \text{ eV} \) and \( d = 156.5 \text{ nm} \). Further details of the calculations in Fig. 3 are given in Supporting Information. For the 2DEG, \( T_{\text{tot}} \) was similar for all scattering potentials studied [Fig. 3(A)–3(C), left], with \( T_{\text{tot}} \rightarrow 1 \) only after \( \frac{d}{\lambda} \geq 1 \) at \( \theta_{k_1} = 0 \). For \( \frac{d}{\lambda} \ll 1 \), there was negligible transmission of the incident wave in the 2DEG for all \( \theta_{k_1} \). In graphene, however, the dependence of \( T_{\text{tot}} \) on \( \frac{d}{\lambda} \) and \( \theta_{k_1} \) in Fig. 3 (right) was sensitive to \( V_0 \).

For \( \frac{d}{\lambda} \ll 1 \) and \( \theta_{k_1} = 0 \), \( T_{\text{tot}} \approx 1 \) in all cases as a result of Klein tunneling as previously illustrated in Fig. 2. However, for \( \theta_{k_1} \neq 0 \), specular reflection can occur leading to \( T_{\text{tot}} < 1 \) even for \( \frac{d}{\lambda} \ll 1 \). Again, above \( \frac{d}{\lambda} \geq 1 \), the incident wave can backscatter along the Bragg directions, thereby leading to a reduction in \( T_{\text{tot}} \) even at normal incidence.

In Fig. 3, sharp features in \( T_{\text{tot}} \) (indicated by * in Fig. 3) were also observed around the following values of \( \frac{d}{\lambda} \) in graphene: [Fig. 3(B), right] \( \frac{d}{\lambda} = 1.6915 \) for \( V_0 = 0.8 \text{ eV} \), [Fig. 3(A), right] \( \frac{d}{\lambda} = 0.8887 \) for \( V_0 = 0.2 \text{ eV} \), and [Fig. 3(C), right] \( \frac{d}{\lambda} = 1.3 \) for \( V_0 = -0.9683 \text{ eV} \). These sharp changes in \( T_{\text{tot}} \) appear to result from the interference between partial waves from the individual scatterers at values of \( k_1 d \) where \( s_j \rightarrow -1 \) for at least one of the higher partial waves with \( l \geq 2 \) while at the same time \( |s_j| \in [0.8, 1] \) and/or \( |s_j| \in [0.8, 1] \). Approximate values for these \( k_1 d \) where \( s_j \rightarrow -1 \) can be determined from \( s_j \) [Eq. (6)] and are solutions to the following equation:

\[
J_{l+1}(k_1 r_s) Y_l(k_1 r) - J_l(k_1 r_s) Y_{l+1}(k_1 r) = 0
\]

where \( Y_l(z) \) is a Bessel function of the second-kind. In Figure 3, the interference between the \( l = 0 \) and \( l = 2 \) partial waves was observed in Fig. 3(A) and Fig. 3(C) at \( \frac{d}{\lambda} = 0.8887 \) \( |s_0| = 0.9355 \) and \( |s_2| = 0.9999 \) and \( \frac{d}{\lambda} = 1.18725 \) \( |s_0| = 0.8863 \) and \( |s_2| = 0.9994 \), respectively, whereas the interference between the \( l = 0, l = 1 \), and \( l = 3 \) partial waves was observed in Fig. 3(B) at \( \frac{d}{\lambda} = 1.6915 \) \( |s_0| = 0.7964 \) \( |s_1| = 0.8005 \) and \( |s_2| = 1 \). Note that a similar interference between higher partial waves was also observed in the 2DEG near \( \frac{d}{\lambda} = 1.50225 \) [Fig. 3(C), left] with an attractive scattering potential, \( V_0 = -0.9683 \text{ eV} \), which was a result of the interference between the \( l = 0 \) and \( l = 3 \) partial waves \( |s_0| = 0.9436 \) and \( |s_2| = 0.8609 \). Furthermore, calculations of \( T_{\text{tot}} \) in the 2DEG using the scattering amplitudes in graphene \( |s_j| \) in Eq. (6)] also exhibited sharp features in \( T_{\text{tot}} \) at the same values of \( k_1 d \) (data not shown). The effects of partial interference between higher partial waves that suppress forward scattering have been previously noted in graphene and for Mie scattering in optical systems.

**Discussion**

A theory for scattering of electron waves incident to a one-dimensional array of localized cylindrically symmetric scatterers [Figure 2(A)] in graphene was used to study the transmission probability through the scattering array as a function of angle of incidence, \( \theta_{k_1} \), and wavelength \( \lambda \) [see Supporting Information for a derivation of the theory]. When the spacing between scatterers, \( d \),...
for the range of $d$ given by $d < \frac{\sqrt{2}}{200\pi} \cdot \frac{\sqrt{\pi}}{2}$. In a (left) 2DEG and in (right) graphene for following scattering potentials and lattice spacings: (A) $V_0 = 0.8$ eV $[l_{\text{max}}$ ranging up to $l_{\text{max}} = 4$ in both graphene and the 2DEG] and $d = 150$ nm, (B) $V_0 = 0.2$ eV $[l_{\text{max}}$ ranging up to $l_{\text{max}} = 4$ in both graphene and the 2DEG] and $d = 150$ nm, and (C) $V_0 = -0.9683$ eV $[l_{\text{max}}$ ranging up to $l_{\text{max}} = 6$ for graphene and $l_{\text{max}} = 4$ for the 2DEG] and $d = 156.5$ nm. In Figs. 3(A) and 3(B), the wave vector within the scattering potential was given by $k_0 = k_x + \frac{|V_0|}{\hbar v_F}$ in graphene and $-i k_x$ in the 2DEG since $k_x < \frac{\hbar}{v_F}$ for the range of $d$ plotted in Figs. 3(A) and 3(B). In Fig. 3(C), the wave vector inside the scattering potential was given by $k_2 = k_x + \frac{|V_0|}{\hbar v_F}$ in both graphene and the 2DEG. Asterisks (*) denote those values of $d$ where interference between higher partial waves from the individual scatterers generate sharp features in $T_{\text{tot}}$ [Eq. (4)].

Methods

The theory for scattering of a massless Dirac plane wave spinor from a one-dimensional array of localized cylindrically symmetric scatterers [Fig. 1(B)] is developed in Supporting Information S3-5, where it is shown that the full scattering solution for $\psi_{\text{tot}}(r)$ incident to the scattering array shown in Fig. 1(B), $\psi_{\text{tot}}(r)$, can be written as [for $x \neq 0$]:

$$
\psi_{\pm r}(r) = \psi_{\pm r}(r) + \sum_{l=0}^{l_{\text{max}}} \sum_{n,m=1}^{k_{n}} \frac{2i^{l+n}}{k_{l_{n}l_{m}}} \left( \mp \text{sign}(x) \right) \left( \frac{\sinh(n \pi l_{n})}{\sinh(n \pi l_{m})} \right) \left( \frac{\sinh(n \pi l_{n})}{\sinh(n \pi l_{m})} \right) \frac{\sinh(n \pi l_{n})}{\sinh(n \pi l_{m})}
$$

In all simulations, each scatterer was modeled as a cylindrically symmetric barrier/ well of potential $V_0$ and radius $r_s$. For an individual scatterer, the $p$th partial wave scattering amplitude is given by $A_{l,p}$:

$$
\psi_{l_{n}l_{m}} = k_{l_{n}l_{m}} + \frac{2i^{l+n}}{k_{l_{n}l_{m}}} \text{ for } k_{l_{n}l_{m}} \geq k_{l_{n}l_{m}} \text{ and }\text{ for } k_{l_{n}l_{m}} < k_{l_{n}l_{m}} \text{ is imaginary.}
$$

In all simulations, an infinite number of partial waves that are included in the calculations, $k_{l_{n}l_{m}} = k_{l_{n}l_{m}} + \frac{2i^{l+n}}{k_{l_{n}l_{m}}}$. For $k_{l_{n}l_{m}} \geq k_{l_{n}l_{m}}$ or $k_{l_{n}l_{m}} < k_{l_{n}l_{m}}$, the $k_{l_{n}l_{m}}$ and $k_{l_{n}l_{m}}$ are first-order Bessel and Hankel functions of order $l$, respectively. The maximum partial wave used in the calculations, $l_{\text{max}}$, was chosen to take into account 99.9% of the total scattering amplitudes for an individual scatterer, i.e., $\sum_{l=0}^{l_{\text{max}}} |A_{l,p}|^2 = 0.999 \sum_{l=0}^{\infty} |A_{l,p}|^2$.

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Figure 3 | Total transmission probability, $T_{\text{tot}}$, for a plane wave incident to an infinite one-dimensional array of localized cylindrically symmetric scatterers of radius $r_s = 20$ nm as a function of incident angle, $\theta_{i_{n}} \in [0.1 \pi, 0.9 \pi]$, and the ratio of lattice spacing to wavelength, $d_{l_{n}} \in [200 \pi, 180 \pi]$, in a (left) 2DEG and in (right) graphene for out scattering potentials and lattice spacings: (A) $V_0 = 0.8$ eV $[l_{\text{max}}$ ranging up to $l_{\text{max}} = 4$ in both graphene and the 2DEG] and $d = 150$ nm, (B) $V_0 = 0.2$ eV $[l_{\text{max}}$ ranging up to $l_{\text{max}} = 4$ in both graphene and the 2DEG] and $d = 150$ nm, and (C) $V_0 = -0.9683$ eV $[l_{\text{max}}$ ranging up to $l_{\text{max}} = 6$ for graphene and $l_{\text{max}} = 4$ for the 2DEG] and $d = 156.5$ nm. In Figs. 3(A) and 3(B), the wave vector within the scattering potential was given by $k_0 = k_x + \frac{|V_0|}{\hbar v_F}$ in graphene and $-i k_x$ in the 2DEG since $k_x < \frac{\hbar}{v_F}$ for the range of $d$ plotted in Figs. 3(A) and 3(B). In Fig. 3(C), the wave vector inside the scattering potential was given by $k_2 = k_x + \frac{|V_0|}{\hbar v_F}$ in both graphene and the 2DEG. Asterisks (*) denote those values of $d$ where interference between higher partial waves from the individual scatterers generate sharp features in $T_{\text{tot}}$ [Eq. (4)].

is much less than $\frac{d}{\lambda} < 1$, the scattering array in Fig. 2(A) acts like a continuous one-dimensional potential barrier/ well [Fig. 1(A)]. In this case, electron waves normally incident to the scattering array are perfectly transmitted as a consequence of Klein tunneling.15,19. However, when $\frac{d}{\lambda} \geq 1$, the incident electron waves are able to “resolve” the fact that the scattering array is made up of discrete, localized scatterers that can reflect the incident electron wave along the Bragg directions that do not correspond to direct backscattering [Fig. 1(B)]. As a result, the transmission probabilities can be significantly less than one when $\frac{d}{\lambda} \geq 1$, even at normal incidence [Fig. 2]. In effect, placing periodic openings into a constant one-dimensional potential barrier/well can, somewhat counterintuitively, reduce the transmission probability at normal incidence, i.e., suppress Klein tunneling, in graphene. It was demonstrated [Fig. 3, right] that the dependence of the transmission probabilities on incident angle, $\theta_{i_{n}}$, and electron wavelength was more sensitive to the scattering potential in graphene relative to that observed for a regular two-dimensional electron gas (2DEG). Furthermore, when $\frac{d}{\lambda} \rightarrow 1$ for at least one higher partial wave with $l' = 2$ while $|x| \approx |x|$ and/or $|y| \approx |y|$, the interference between the partial waves from the individual scatterers resulted in sharp features in the transmission probabilities [Fig. 3, right].

Similar features were also observed in the transmission probability for a 2DEG with an attractive scattering potential [Fig. 3(C), left]. While only a one-dimensional periodic array of localized scatterers was considered in this work, any potential that has spatial variations larger than the incident electron wavelength will generate non-specular or diffuse reflection that will suppress Klein tunneling. Such potentials could be useful in realizing future graphene electronic devices, such as a graphene field effect transistor.25. Finally, the results presented in this work could be applied to other physical systems that behave like massless Dirac fermions, such as the surface states of topological insulators,23–25, optical analogues of graphene,26, and trapped ions27.
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