Tunable wavevector filtering in borophane based normal metal-barrier-normal metal junctions

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Abstract
We study the transport properties of Dirac electrons across a two-dimensional normal metal-barrier-normal metal interface in monolayer borophane. We analyse the transmission probability with variation of the width of the barrier region, the incidence energy and transverse momentum. We demonstrate that a gap exists in the transmission probability spectrum and the position of the width of the transmission gap can be tuned by the barrier strength and transverse momentum respectively. We point out the variation of the ballistic tunneling conductance as a function of the width of the barrier region and incident energy. We find that the oscillatory or decaying nature of the conductance with variation in barrier width depends upon the number of propagating and evanescent modes which are controlled by the incident energy and barrier strength. We show that the conductance as a function of incident energy drops to a minimum value when the incident energy becomes identical to the barrier height and identify that this effect is caused by the presence of evanescent modes inside the barrier. Based on these findings we propose a perfectly tunable wavevector filter for borophane. We expect our findings possess useful applications in borophane based nano-electronic devices.

Keywords: borophane, transmission probability, wavevector filtering, normal metal-barrier-normal metal junction, propagating modes, evanescent modes, ballistic conductance

(Some figures may appear in colour only in the online journal)

1. Introduction

Over the last decade, after the discovery of graphene [1], two-dimensional Dirac materials [2–6] such as graphene and topological insulators [7] appear to be a subject of intriguing interest in both theoretical and experimental condensed matter physics. The low-energy quasiparticles of such two-dimensional materials behave as relativistic Dirac particles [8–12] and henceforth the materials exhibit numerous exotic signatures like the unconventional quantum Hall effect [13–16], minimum conductivity [14], the unusual Kondo effect [17–21], exceptional transport properties [22–26] etc.

Borophane is one such two-dimensional material, fabricated from boron. Among various nanostructures of boron, a 2D graphene-like crystal called borophane has been investigated extensively [27–29] due to its unconventional asymmetry feature compared to graphene. The honeycomb lattice structure of boron is unstable due to electron deficiency. However, a stable lattice structure can be obtained with the introduction of additional boron atoms. This leads to many possible allotropes such as α sheet, β sheet, β12 sheet, 8-Pmnn borophene etc. Signatures of anisotropic massless Dirac Fermions have been exhibited in the β12 sheet [30] and also in the 8-Pmnn borophene [31]. The presence of imaginary frequencies in
the phononic dispersion of borophene leads to instability of the material against the periodic vibrations with long wavelengths \cite{32,33}. Surface hydrogenation of borophene is one feasible method to construct stabilised borophene. According to Xu et al \cite{32}, fully hydrogenated borophene (B$_2$H$_2$), called borophane, is a stable structure which is produced in vacuum without adding a substrate to borophene. The behaviour of borophane as Dirac material with a remarkable Fermi velocity, twice to four times of that of graphene, is also exhibited \cite{32,34,35}. Density functional theory (DFT) calculations show the existence of an anisotropic tilted Dirac cone in borophane \cite{32,36}. The anisotropy feature of borophane is also manifested in its mechanical properties \cite{37–39}, electrical properties \cite{40,41}, magnetic properties \cite{42–44}, optical properties \cite{45,46} and superconductivity \cite{47–50}. Along the valley direction (armchair), the current–voltage characteristic of borophane is linear showing a metallic trend in contrast to the buckled direction, exhibiting semiconductor nature \cite{51–53}.

The presence of such anisotropy along with the tilt in the material with a high Fermi velocity motivates us to study whether the tilt affects the transport properties. The ballistic normal metal-barrier-normal metal (NBN) junction is the basic constituent of various novel devices, in which Dirac Fermions exhibit a lot of unusual features and provides a platform to study the transport properties. A completely different nature between Dirac and Schrödinger quasiparticles can be explored using NBN junctions. Although the barrier strength has a higher value than incident energy, the transmission probability in NBN junction and the conductance show oscillatory nature for Dirac like quasiparticles in contrast to the exponentially decaying nature of Schrödinger quasiparticles.

In this work, we have studied the transport properties of Dirac electrons in borophane across a NBN junction. Since the tight binding Hamiltonian of borophane possesses anisotropy in momentum space, the orientation of the NBN junction should have an important effect in the transport properties. The presence of the linear $k_z$ term (tilt) in dispersion relation stimulates us to choose the orientation of the junction along the $\Gamma-X$ direction. Our motivation is to explore how the tilted dispersion affects the formalism and hence the transport properties of a NBN junction in borophane. We have found that the presence of a tilting term in the Hamiltonian has a considerable effect on the formalism of transport. One unique feature to emphasise is that an anisotropy is introduced between the angle of reflection and the angle of incidence. The isotropic case of mirror reflection is modified in this case and the formalism reduces to that of isotropic non-tilted material such as graphene as a limiting case when the tilt term vanishes. We have analytically studied the transmission probability and then the ballistic tunneling conductance is found out numerically. As already stated, in the limit when the tilt term vanishes, our result agrees with that of graphene, as expected. We find that the transmission probability is an oscillatory or a decaying function of the barrier width depending upon the incident energy, barrier strength and the transverse momentum. We have presented a condition of transition between these two phases and the phases are shown in a phase diagram as a function of a critical parameter. The conductance also exhibits the transition from oscillatory to decaying region as a function of barrier width. There exists a transmission gap in the transmission spectrum due to the presence of evanescent modes within the barrier. The appearance of evanescent modes leads to minima in the conductance spectrum. We have investigated the modulation of transmission gap by varying the model parameters like the incident energy, barrier strength and the transverse momentum. We present a discussion on how the nature of conductance depends on the nature and number of contributing transmission modes if one varies incident energy and barrier strength. Our results show that one can effectively design a tunable wavevector filter \cite{54–59} using a borophane based NBN junction.

The rest of the paper is organised as follows. In section 2, we explain the model, formalism and the analytical calculation of transmission probability starting from low energy effective Hamiltonian of borophane. Then in section 3, we have discussed our analytical and numerical results. Lastly, we conclude and abridge our findings in section 4.

2. Model and formalism

In this section, we study the ballistic transport of Dirac electrons across a normal NBN junction in borophane, as shown in figure 1. Since borophane possesses lower crystal symmetry, in contrast to graphene, the low-energy effective Hamiltonian contains asymmetric velocity parameters which results in the two tilted Dirac cones at the Dirac points $\mathbf{k}_0 = (\pm 0.64, 0) \ \text{Å}^{-1}$ \cite{60–64}. The unit cell of the borophane contains four atoms and the Bravais lattice constants are $(a_x, a_y) = (1.92, 2.81) \ \text{Å}$ \cite{63} as shown in figure 2.

The low-energy effective Hamiltonian for normal borophane in the vicinity of the Dirac point is given by \cite{63}

$$H_0 = \hbar \sum_{\mathbf{k}} \psi^\dagger_\mathbf{k} \begin{bmatrix} v_x k_1 \sigma_x + v_y k_2 \sigma_y + v_z k_3 \sigma_0 \end{bmatrix} \psi_\mathbf{k}$$

(1)

where $\psi_\mathbf{k} = (a_\mathbf{k}, b_\mathbf{k})^T$, here $a_\mathbf{k}$ and $b_\mathbf{k}$ stands for the annihilation operators of the Bloch states of the two triangular sublattices in borophane. $\sigma_{0, x, y}$ represents usual two dimensional identity and Pauli matrices for the pseudospin space respectively. The Hamiltonian describes an anisotropic 2D tilted Dirac cone, specified by $v_x$, $v_y$ and $v_z$, the velocities in
the $x$ and $y$ directions and the degree of tilting in the $x$ direction respectively. Typical values for the velocities, in units of $(\times 10^3 \text{ m s}^{-1})$, are $v_x = 19.58$, $v_y = 6.32$ and $v_z = -5.06$. Diagonalization of the Hamiltonian gives the energy spectrum

$$E_{s,k} = \hbar \left[v_x k_x + s \sqrt{(v_x k_x)^2 + (v_y k_y)^2}\right]$$  \hspace{2cm} (2)

where $s = \pm 1$ denotes the conduction and valence band respectively. The energy dispersion is shown in the three dimensional plot in figure 3(a). The corresponding eigenvectors are

$$\psi_k = (1, s \exp[i \beta_k])^T / \sqrt{2},$$

$$\tan(\beta_k) = \frac{v_y k_y}{v_x k_x} = \frac{v_y}{v_x} \tan(\phi_k)$$  \hspace{2cm} (3)

where $s = \text{Sgn}(E - \hbar v_x k_x)$ and $\text{Sgn}$ denotes the signum function. Here the angle $\phi_k$ specifies the direction of $k$ with respect to $k_x$ axis in the momentum space. Due to the presence of the tilting term, the Hamiltonian is not symmetric under the parity operation $k_x \rightarrow -k_x$ and the Fermi surface is not a circle. For a fixed energy $E_{s,k}$, the equation determining the Fermi surface can be written as

$$\frac{(k_x - k_{s,c})^2}{k_{s,a}^2} + \frac{k_y^2}{k_{s,b}^2} = 1,$$

where

$$k_{s,c} = \frac{E_{s,k} |v_x|}{\hbar |A|}, \quad k_{s,a} = \frac{E_{s,k} v_x}{\hbar |A|},$$

$$k_{s,b} = \frac{E_{s,k} v_y}{\hbar v_x \sqrt{|A|}}, A = v_y^2 - v_x^2 < 0.$$

Equation (4) represents an ellipse with center at $(k_{s,c},0)$, shifted along $x$ direction. Since the center of the ellipse $k_{s,c} \propto E_{s,k}$, the Fermi surface for conduction and that for valence band are shifted in different way. The Fermi surface for conduction (valence) band is a shifted ellipse along the $+(-)x$ direction.

Figure 2. Schematic illustration of borophane lattice structure exhibiting top view, side view and front view. The unit cell is shown as the black rectangle which contains two boron atoms (red balls) and two hydrogen atoms (aqua balls). Here $a_x$, $a_y$ represents the primitive lattice constants along $x$ and $y$-directions, respectively.

Figure 3. Upper panel (a) plot of the anisotropic, tilted energy band dispersion of borophane in the vicinity of $k_D$ point, in the $k_x$-$k_y$ plane. Lower panel (b) plot showing Fermi surface for conduction band (CB) and valence band (VB) respectively. The Fermi surfaces are tilted along $\pm x$ direction for CB and VB accordingly, with the ratio of semi-minor and semi-major axes being identical for both the bands. Representing values on the contours are in eV.
as shown in figure 3(b). But the ratio of semi-minor and semi-major axes \( k_{x,0}/k_{x,\alpha} = \sqrt{(\nu_f^2 - \nu_0^2)}/\nu_c \sim 3 \), being independent of band index \( s \), remains identical for both of the bands and is a characteristic property of the material borophane.

In the presence of barrier, the Hamiltonian can be written as

\[ \mathcal{H} = \mathcal{H}_0 + U \]  

(5)

where the last term \( U \) represents the barrier potential contribution from the external field. Electrons with an energy \( E = \mu + eV \) where \( \mu \) is the chemical potential and \( V \) is the applied bias voltage are incident upon the barrier.

We shall focus on the transport in the \( x \) direction and henceforth assume that the system is translationally invariant along the \( y \) direction. The parallel momentum \( k_x \) for the electron with incident energy \( E \) and conserved transverse momentum \( q \) can be determined from the solution of the following relation

\[ A k_x^2 + B k_x + C = 0 \]  

(6)

where \( B = 2|\nu|E/h \) and \( C = (E/h)^2 - \nu^2 q^2 \). We note that since the equation (6) admits two solutions for \( k_x \), corresponding to any given energy \( E \) and transverse momentum \( q \), we have to identify the propagating right moving mode as the incident one. This is achieved by requiring the right (left) moving modes to be finite when \( x \to \infty \) \((x \to -\infty)\) \[65\]. Substituting \( E = E + i\eta \) in equation (6) with \( \eta \) being an infinitesimally small positive number, one can identify the right (left) moving mode as the complex root with small \( +ve \) \((-ve\)) imaginary part. Also the condition for the solution of equation (6) to be real in the normal metal region (region I: \( x < 0 \), as shown in the figure 1) restricts the ratio of incident energy \( E \) and transverse momentum \( q \) to follow the relation

\[ (E/hq)^2 > \nu_0^2; \quad \nu_0^2 = |A|\nu^2/\nu_c^2. \]  

(7)

To study the transport properties, we shall focus on the electrons in the conduction band in the region I. The wavefunctions in the NBN regions \( \psi(x)e^{i\phi} \) can be read off from equation (3) and are given by

\[ \psi_L(x) = \frac{1}{\sqrt{2}} \left( e^{i\alpha x} + \frac{r}{\sqrt{2}} e^{i\alpha_R x} \right) e^{i|\nu| x}, \]

\[ \psi_R(x) = \frac{p_1}{\sqrt{2}} \left( e^{i\alpha_R x} + \frac{r}{\sqrt{2}} e^{i\alpha_L x} \right) e^{i|\nu| x}, \]

\[ \psi_{II}(x) = \frac{1}{\sqrt{2}} \left( e^{i\alpha x} + \frac{r}{\sqrt{2}} e^{i\alpha_R x} \right) e^{i|\nu| x} \]  

(8)

where \( k_{RL}(k'_{RL}) \) are the right and left moving parallel wavevectors in region I (II) and are given by the solution of equation (6) \((E \) replaced by \( E - U_0 = \delta \), \( \delta = \text{sgn}(E - U_0 - hv_kk'_{RL}) \), \( \alpha_{RL} \equiv \alpha_{RL}(k, k') = \beta(k_{RL}, q) \) and \( \alpha'_{RL}(k) = \beta(k_{RL}, q) \). Here \( r, p_1, p_2 \) and \( \eta \) denote the reflection and transmission coefficients at the first and the second interface and can be found out from the boundary conditions of matching the wavefunctions at the interfaces \( x = 0 \) and \( x = d \). We have omitted the subscript from \( \alpha (\alpha') \) denoting the dependence on the wavevector for brevity and use this notation throughout. One point to mention that the angle of incidence \( \phi_L \) and the angle of reflection \( \phi_R \) for each interface are related to the angles \( \alpha(\alpha') \) as evident from equation (3) such as

\[ \tan \alpha_{RL} = \tan \beta(k_{RL}, q) = \frac{v_L q}{v_L k_{RL}} = \frac{v_L}{v_c} \tan(\phi_{RL}), \]

\[ \tan \alpha'_{RL} = \tan \beta(k'_{RL}, q) = \frac{v_L q}{v_L k'_{RL}} = \frac{v_L}{v_c} \tan(\phi'_{RL}). \]  

(9)

The unique asymmetry feature of borophane is reflected in the right and left moving parallel momenta \( k_{RL} \) and accordingly in the angle of reflection \( \phi_R \) and the angle of incidence \( \phi_L \). For graphene with higher symmetry in contrast to borophane, the right and left moving parallel momenta \( k \) for each interface are related via \( k_L = -k_R \) and correspondingly \( \alpha_L + \alpha_R = \phi_L + \phi_R = \pi \). This is not valid for borophane which indicates that the angle of reflection and the angle of incidence for each interface in case of borophane NBN junction do not follow the rule of mirror reflection. Such unconventional feature is unique to the tilted Hamiltonian. The tilting effect modifies the transmission compared to that of isotropic case which is evident in the detail form of the final transmission coefficient given by

\[ t = \frac{e^{i(k_{RL}^d - k_{RL}^d)}(e^{i\alpha_R} - e^{i\alpha_L})e^{-ik_{RL}^d}}{D_1}, \]

\[ D_1 = \frac{\Delta k_{RL}^d}{2} \left( e^{i(\alpha'_{RL} + \alpha_{RL})} + e^{i(\alpha'_{RL} + \alpha_{RL})} - e^{ik_{RL}^d} \left( e^{i(\alpha'_{RL} + \alpha_{RL})} + e^{i(\alpha'_{RL} + \alpha_{RL})} \right) - s' \left( e^{ik_{RL}^d} - e^{ik_{RL}^d} \right) \right) \left( e^{i(\alpha'_{RL} + \alpha_{RL})} + e^{i(\alpha'_{RL} + \alpha_{RL})} \right). \]  

(10)

Transmission probability is computed as

\[ T = t^* \left[ \mathcal{N} D^2 + \mathcal{D} \mathcal{N} \right] = 4 \sin^2 \left( \frac{\alpha'_{RL} - \alpha'_{RL}}{2} \right) \sin^2 \left( \frac{\alpha_{RL} - \alpha'_{RL}}{2} \right), \]

\[ D = \mathcal{N} + 2 \sin^2 \left( \frac{k_{RL}^d - k_{RL}^d}{2} \right) [1 + \cos(\alpha'_{RL} + \alpha_{RL}) \cos(\alpha_{RL} + \alpha_{RL}) + \sin(\alpha'_{RL} + \alpha_{RL}) \sin(\alpha_{RL} + \alpha_{RL}) + \cos(\alpha'_{RL} - \alpha_{RL}) + \cos(\alpha'_{RL} - \alpha_{RL}) + \cos(\alpha'_{RL} - \alpha_{RL})]. \]  

(11)
Figure 4. Plot of the transmission probability $T_{\text{thin}}$ as a function of effective barrier strength $\chi$ for several values of $E$ with $q = \pi$ (in units of $\text{Å}^{-1}$). Here $E$ (in eV) = 13 (blue solid line), 16.5 (red dotted line) and 33 (black dashed line). The plot shows oscillatory behavior.

Equation (11) reproduces the formula for transmission probability of Dirac electrons in case of graphene based NBN junction [66] by imposing the condition on the parallel momenta (in the limit $v_f \to 0$) such as $k_L(k'_g) \rightarrow -k_R(-k'_g)$.

$$T_{\text{graphene}} = \frac{\cos^2 \alpha_R \cos^2 \alpha'_R}{\cos^2 \alpha_R \cos^2 \alpha'_R \cos^2 k'd + \sin^2 k'd(1 - \sin \alpha_R \sin \alpha'_R)^2}.$$  

(12)

In the thin barrier limit $U_0 \to \infty$, $d \to 0$ with finite value of $U_0d$, the transmission probability is reduced to

$$T_{\text{thin}} = \frac{1}{\cos^2 \chi + \gamma^2 \sin^2 \chi}, \quad \gamma = \frac{\sin(\frac{\alpha_f + \alpha_s}{2})}{\sin(\frac{\alpha_f - \alpha_s}{2})}$$  

(13)

where $\chi = v_f U_0d/h|A|$ is the effective barrier strength.

The ballistic conductance for the system is obtained using Landauer–Büttiker’s formula [67]

$$G(E) = G_0 \int_{-q_{\text{max}}}^{q_{\text{max}}} \frac{dq}{2\pi} T(E, q)$$  

(14)

where $G_0 = e^2 L_y/h$, $L_y$ being the system size along $y$ direction and $q_{\text{max}} = E/(h|V_0|)$ denotes the maximum transverse momentum obeying the relation (7). This has been evaluated numerically. The existence of a cut-off in momentum ($q_{\text{max}}$) is due to the constraint of the incident parallel momentum in normal regions needing to be real. For a fixed energy, $k_x$ in normal region is real for only some of the values of the transverse momentum $q$, as evident from equation (6). This in turn limits the number of momentum modes contributing to the conductance for a particular value of incidence energy.

3. Results and discussion

In this section, we shall chart out the results of the corresponding theory for transport of Dirac electrons in borophane through a single barrier along $x$ direction, developed in section 2. Figure 4 shows the dependence of transmission probability in thin barrier limit on the effective barrier strength for electrons with a finite transverse momentum and different incident energies. We note that an electron with higher incident energy crosses the barrier with a greater transmission probability for a specific value of barrier strength, as expected. Also for $\chi \rightarrow n\pi$ ($n = 1, 2, 3, ...$), the barrier is always transparent ($T_{\text{thin}} \rightarrow 1$), irrespective of the incident energy of the electrons. Another interesting point is that the periodicity in $T$ is independent of the incident energy because $E/U_0 < \pi$ and $U_0$ determines the energy scale of the system.

To discuss the variation of transmission probability as a function of barrier width $d$, we find that the transmission probability may be oscillatory or decaying depending upon the parallel momentum in region II. With real value of $k'_g$, $T$ is oscillatory which is due to the interference effect between the incident and reflected wave in region II. If the interference happens to be constructive, the transmission displays resonances, known as Fabry–Perot resonance. As evident from equation (11) that the condition for Fabry–Perot resonance is $(k'_R - k'_L)d = 2n\pi$ ($n = 0, 1, 2, 3, ...$). On the other
hand the evanescent waves are present in the barrier region for imaginary value of $k'$ and then the transmission probability is exponentially decaying. The decaying behaviour is known as tunneling effect. The condition for appearance of evanescent waves in the barrier region is

$$\langle E - U_0 \rangle^2 - (\hbar v_0 q)^2 < 0$$

Thus the transition between the above mentioned oscillatory and decaying modes can be presented in terms of a critical transverse momentum $q_c = |E - U_0|/(\hbar v_0) = |\delta|/(\hbar v_0)$. The critical momentum is shown in the figure 5, termed as phase diagram, plotted in the $(\delta/\hbar, q)$ plane. For $|lq| < q_c$, the region is oscillatory and on the other hand for $|lq| > q_c$, the region contains evanescent waves. The two regions (propagating and evanescent) are separated by the critical momentum line $q = q_c$. The plot being symmetric under $\delta \rightarrow -\delta$, it is evident that for same value of $|\delta|$, the transmission probability must display identical nature irrespective of $E < U_0$ or $E > U_0$.

In the figure 6, transmission probability with different incident energy and fixed values of transverse momenta and barrier strength is plotted against the barrier width. As evident from the phase diagram figure 5, while $|lq| < q_c$, the electrons can propagate through the potential barrier (as shown for $E = 4.3$ eV and $E = 18$ eV in figure 6 and in the other cases, they decay exponentially inside the barrier. For propagating mode, the characteristics of oscillation depend on $E$ for a fixed $U_0$ and $q$, unlike the thin barrier limit. With increase in energy, the period of oscillation increases and amplitude decreases as shown for 4.3 and 18 eV. For $E \gg U_0$ (as shown with $E = 30$ eV case), the amplitude of oscillation decreases significantly and the barrier is nearly transparent irrespective of the barrier width. For the tunneling modes, decay of $T$ depends upon the difference between the incident energy and barrier strength $|\delta|$ as $1/T \sim \sinh^2(\sqrt{|\hbar v_0 q|^2 - \delta^2})$. Hence for small value of $|\delta|$, the decay of $T$ would be sharper with $q$ being fixed, as shown in $E = 13.3$ eV case.

One signature of a Dirac Fermionic system is reflected in the dependence of the transmission on the critical momentum $q_c$. Due to the dependence of $q_c$ on $|E - U_0|$ for borophane, as pointed out before, it may happen that though $E < U_0$, $T$ is oscillatory (shown by the blue solid line for $E = 4.3$ eV and $U_0 = 13.3$ eV) and alternatively for $E > U_0$, $T$ is decaying (shown by the black dashed line for $E = 13.3$ eV and $U_0 = 13.2$ eV). Thus the ratio $E/U_0$ does not play the determining role for transmission to be oscillatory or decaying, in contrast to the case of Schrödinger quasiparticles.

The presence of evanescent modes leads to a gap in transmission probability determined by the conditions $q^2 < q_c^2$. The appearance of the transmission gap is shown in figure 7. In figure 7, the dependence of transmission probability on the incident energy and transverse momentum is studied for a fixed value of the barrier strength and barrier width. Unimpeded penetration at normal incidence $q = 0$, known as Klein paradox, is obtained. Then the barrier is fully transparent at any values of incident energy, barrier strength or barrier width. This is the unique signature of any Dirac Fermionic system. As discussed, the existence of the evanescent waves in the
We mention that, as already discussed, decaying nature are clearly seen in the plot. Another point to note for a particular value of incident energy and barrier strength, the number of momentum modes contributing to the conductance are finite. We have studied such situations in two ways, formerly keeping the number of contributing modes \((n_p + n_e)\) fixed (tuning \(\delta\)) and then with a fixed \(n_p\) (changing \(E\) and \(U_0\), keeping \(|\delta|\) fixed). At a fixed \(E\), \((n_p + n_e)\) gets determined as in figure 9. We recognise that the modes with specific value of transverse wave vector are transmitted for a particular value of incident energy and barrier strength. Again, with identical \(|\delta|\) \((U_0 = 5 eV and 57 eV)\), the number of modes are same. The number is smallest for \(\delta = 0\). We note that the number of transmitted (propagating) modes is quite independent of the barrier width. This enhances the understanding of the filtering action of borophane.

To study the nature of ballistic conductance, we plot the conductance against the width of the barrier and incident energy. We want to emphasise that while averaging over transverse momentum in computing ballistic conductance, one have to impose a limit on \(q\). This in turn restricts the number of momentum modes contributing in the conductance. The incident energy via \(q_{\text{max}}\) determines this number of modes. Interplay between the incident energy and barrier strength controls the nature of contributing modes. The number of propagating (oscillatory) and evanescent (tunneling) modes \((n_p, n_e)\) occupies a significant role to determine the nature of the conductance. The cut-off in momentum mode \(q_{\text{max}}\) determines the total number of modes contributing to the conductance and thus the total number \((n_p + n_e)\) is proportional to \(2q_{\text{max}} = 2E/\hbar v_0\). On the other hand, the number of propagating modes \(n_p\) is proportional to \(2q_{c} = 2|E - U_0|/\hbar v_0\) because whenever \(-q_{c} \leq q \leq q_{c}\), the modes are oscillating. Thus depending upon the values of \(E\) and \(U_0\) \((n_p, n_e, \text{and } q_{\text{c}}\) change accordingly), two types of phenomena determine the nature of the conductance. We can identify two zones depending upon the value of the ratio \(|\delta|/E\) which is also evident in the phase diagram figure 5. For smaller value of \(|\delta|/E\), the propagating modes are few in number and alternatively with increase in \(|\delta|/E\), the number of propagating modes starts to increase. Hence in the first zone with \(|\delta|/E \ll 1\), quantum tunneling through evanescent modes is predominant \((n_e > n_p)\) and hence the conductance as a function of barrier width should decay and reaches to a minima. The value of the conductance minima is lowest for \(\delta = 0\) when \(n_p\) is smallest due to filtering effect. On the other hand, with increase in \(|\delta|/E\), \(n_e\) decreases and in turn the value of the minima increases. If \(|\delta|/E\) is increased further \((n_p\) becomes comparable to \(n_e\)), Fabry–Perot resonance begins to dominate. While discussing the behaviour in the second zone with large value of \(|\delta|/E\), one can divide the zone into two sub-zones depending on the signature of \(\delta\). Formerly in the first sub-zone with large \(+ve\) values of \(\delta\), \(E > U_0\) and hence the oscillation in transmission probability becomes very weak and the barrier is mostly transparent. This results in the decay of the conductance but the value of the minima being larger than the previous one with smaller \(|\delta|/E\). In the second sub-zone with \(|\delta|/E \ll 0\), \(E \ll U_0\), the oscillation in transmission probability is prominent and hence the conductance displays an oscillatory behaviour. In this case, it may happen that transmission occurs through propagating modes only \((n_e = 0)\) and then the oscillation in the conductance is more pronounced.

We have studied such situations in two ways, formerly keeping the number of contributing modes \((n_p + n_e)\) fixed (tuning \(\delta\)) and then with a fixed \(n_p\) (changing \(E\) and \(U_0\), keeping \(|\delta|\) fixed). At a fixed \(E\), \((n_p + n_e)\) gets determined
for inductance is fairly high, shown in figure 10. With decrease a result the conductance decays and the minima of the conductance drops to a minimum as a result of transmission gap at $E = U_0$.

In figure 11, $|E - U_0| = |\delta|$ is fixed so that $n_p$ remains unchanged while $(n_p + n_e)$ varies. In this case, we need to check the ratio $\delta/E$ to determine the nature of the conductance. Here for $(13.5, 5)$ [(E, $U_0$) in eV], since $\delta/E = 0.6$ and hence the conductance should decay being in the first sub-zone. With $(20, 11.5)[\delta/E = 0.4]$, the decay of conductance is sharper as a result of the suppression in propagating modes. Large oscillation appears for $(5, 13.5)$ because $n_e = 0$ as expected, while for $(11.5, 20)$, the amplitude of oscillation in conductance is relatively low.

The variation of conductance with the incident energy keeping fixed barrier width for different values of $U_0$ is shown in figure 12. We know that a transmission gap centered at $E = U_0$ appears in transmission spectrum as a result of existence of evanescent modes. This causes a suppression in the conductance to a minimum value for $E = U_0$ and position of the minima shifts along the energy axis as $U_0$ is varied. One point to mention that resonance modes in the conductance are present. For $E \leq U_0/2$, only propagating modes are contributing to the conductance ($n_e = 0$) and hence the conductance displays a strong resonance in this region. We note that by changing $U_0$, one can also modulate the width of the strong resonance region in conductance. The period of oscillation in conductance depends upon the barrier width, as expected. Besides, for obvious reasons, the minima of the conductance decreases with the increase of barrier width. Similar feature can be obtained with variation in barrier strength also. Hence we can modulate ballistic conductance by tuning incident energy and barrier strength.

4. Conclusion

In summary, we have investigated the transmission probability and ballistic tunneling conductance of a single layer borophane NBN junction. The tilted nature of borophane, in contrast to graphene, is expressed through the broken mirror symmetry by angle of incidence and angle of reflection and
by the right and left moving parallel momenta in all the regions of NBN junction. We have identified how the tilted term of borophane affects the transmission probability and the conductance. The transmission probability depends on the barrier width, incident energy of the particle, barrier strength and the transverse momentum of the incident particle. We show that there exists a critical value of transverse momentum which in turn determines the nature of transmission probability as a function of barrier width. We present a phase diagram to distinguish the oscillatory and decaying phases in transmission probability in terms of the critical transverse momentum. The transmission probability shows distinguished behaviour as a function of barrier width depending upon whether the transverse momentum is smaller than the critical momentum or not. The analytical expression for the critical momentum has been found. It depends upon the barrier strength, incident energy and the velocities \( v_x \), \( v_y \) and \( v_t \). For \( |q| < q_c \), the electrons are in propagating mode and hence the transmission probability becomes oscillatory while in the other case, it decays exponentially inside the barrier. The nature of transmission probability can be predicted from the ‘phase diagram’, displayed in \((\delta, q)\) plane. While observing the variation of transmission probability with incident energy, we note the existence of a transmission gap. The position and the width of the gap are theoretically calculated. By tuning the parameters like barrier strength or the transverse momentum of the incident particle, filtered transmission may happen. The filtering effect is explicitly evident when we investigate the variation of the transmission probability with the transverse wave vector. We identify that the modes with specific value of transverse wave vector are filtered for a particular value of incident energy and barrier strength and also the number of transmitted modes is quite independent of the barrier width. This enhances the realisation of the tunable wave vector filtering action of borophane. The filtering effect is also shown in the tunneling conductance spectra. The tunneling conductance drops very rapidly when incident energy becomes identical to the barrier strength as a result of the suppression in transmission probability due to evanescent modes. This filtering effect is the central result of our work. There exists a lower and upper bound on the possible contributing transverse momentum modes of the incident particle \((\pm q_{\text{max}})\) while computing the conductance. \( q_{\text{max}} \) is determined by the incident energy and the velocities \( v_x \), \( v_y \) and \( v_t \). The interplay between the Fabry–Perot resonance and the tunneling effect is the determining factor of the nature of conductance as a function of barrier width. This can be expressed through critical momentum and \( q_{\text{max}} \). With a fixed incident energy, the total number of modes, contributing to the conductance, gets fixed and then by varying the barrier strength, the number of propagating (oscillatory) and evanescent (tunneling) modes can be controlled and depending upon their ratio the conductance is oscillatory or in decaying regime. The oscillatory features of tunneling conductance are caused by the interference of the Dirac Fermions in barrier region. Our results clearly demonstrate that the tunneling conductance drops very rapidly in the case when the incident energy varies and the barrier width remains fixed in comparison to the situation of varying barrier width keeping incident energy fixed. As a consequence, it is easier to get prominent filtering effect by tuning the energies like incident energy or the barrier strength rather than by modulating barrier width. Thus the existence of the transmission gap enables to design a tunable wavevector filter in borophane based electronic devices. Due to very fast progress of experimental technologies, we anticipate to observe such wavevector filtering effect of borophane in the near future.

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