The Effect of Twisting Angle on the Electronic Properties and Electron Transport and Hall Effect in the Twisted Circular and Rectangular Graphene and Graphene/Boron-Nitride Channels

Farzaneh Shayeganfar\textsuperscript{1,2,*}, Ali Ramazani\textsuperscript{3,*}, Nicholas X Fang\textsuperscript{3,†}

\textsuperscript{1}Department of Physics and Energy Engineering, Amirkabir University of Technology, Tehran, Iran
\textsuperscript{2}Department of Civil and Environmental Engineering, Rice University, Houston, TX 77005, USA
\textsuperscript{3}Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Abstract: Twisted bilayer graphene (tBLG) including interlayer interaction and rotational disorder shows anomalous electron transport as a function of twist-angles (tAs). In this work, we address the electronic properties and electron transport of circular and rectangular twisted graphene nanoribbon (tGN) and twisted heterostructure of graphene/boron-nitride nanoribbon (thG/BNN) channels by applying the tight-binding Hamiltonian for two regimes of small and large tAs. Analysis of band structure reveals that the circular tGNs for small and large tAs have metallic behavior, while phase transition of metal to semiconductor occurs in rectangular case, sweeping small tAs to large ones. This implies a different transport mechanism depending on the tAs disorder, whiles the Klein paradox appears in the transmission and conductance of circular tGNs. We distinguish that the local electron states of rectangular tGNs with large tAs create degenerate multiflat bands, supporting decoupling of two ribbons and high conductance state. However, coupled two Dirac electron gases for small tAs of rectangular channel cause Klein paradox due to their resonant scattering. We compute the Hall conductivity in both tGNs for wide range of magnetic field. In circular tGNs the valance and conduction band energy is quantized into electron/hole-like Landau level, while for rectangular tGNs with applied magnetic field the Hall conductivity shows complex behavior. Moreover, we provide a platform for quantum transport and Hall effect of thG/BNN, which host a vast nontrivial emergent electronic state. Our findings suggest that circular/rectangular tGNs and thG/BNNs with new electron states of Moiré pattern besides the Klein paradox suitable for switching of several nanochannel.

Keywords: twisted graphene nanoribbons, electron transport, circular and rectangular channel, flat bands, phase transition.

1. Introduction:
Moiré pattern generated by rotation of two honeycomb lattices of bilayer alters the electronic properties of bilayer structure [1-7]. Twisted stacking of two monolayers of graphene with rotation angle couple two Dirac electron gases by a periodic interaction in large supercell. Jarillo-Herrero et al. [6] reported a magic twist-angle (tA) $\theta = 1.1^\circ$ of bilayer graphene, which shows new phase of superconducting. The existence of several small and large angles in graphene multilayers has been observed by angle-resolved photoemission spectroscopy (ARPES) grown on SiC, which is unavoidable in the epitaxial growth and restore graphene like Dirac cones [8,9]. Klein paradox of Dirac electrons due to chirality of their wave function reveals the transparent behavior of Dirac

* Authors have equal contribution.
† Corresponding Author; E-mail: niefang@mit.edu
electrons in potential barrier in one-dimensional structure [10,11]. Therefore, applying the electrostatic potential can challenge localization of Dirac electrons applied in the elementary devices [11,12].

Behavior of Dirac electrons investigated in several types of disordered potentials in epitaxial graphene confirms the lack of backscattering of Klein paradox [13]. Alternatively, periodic interaction of bilayers of graphene creates massive quasiparticles, which reveal the quadratic dispersion near to the Dirac point [4,14]. This rich behavior has been detected in rotated bilayer graphene, where longer period of Moiré pattern is originated from the superposition of the two honeycomb lattices. Laissardie’re et al.[10] reported that localized electrons in rotated graphene bilayers have Fermi velocity close to zero for small \( \theta \), confirming the confinement of Dirac electrons.

More recently, Asano and Nakamura [15] showed that the AA bilayer graphene nanoribbons (GNs) has nonmagnetic edge states, while the AB bilayer GNs exhibits the spin-polarized and includes the magnetic edge states [16,17].

The hybrid graphene/ boron-Nitride (h-BN) forms when monolayer graphene and boron-Nitride (hBN) are stacked together. The graphene/ boron-Nitride (h-BN) bilayer shows bandgap, which changes non-monotonically with \( \theta \) [18]. Such vdW heterostructures possess twist-angle-dependent electronic and optical properties that can extend their application in nano-electronic and optoelectronic devices [19]. From the other side, since the interatomic interaction is fundamentally the electromagnetic force, the change of atomic electronic properties may affect the interatomic force and the lattice structure. [20–23]. Woods et al. [24] reported that the commensurate-incommensurate transition of graphene on the h-BN substrate can increase \( \theta \). At \( \theta < 1^\circ \), the graphene lattice stretches locally to match the h-BN lattice. At \( \theta > 1^\circ \), the graphene and h-BN lattices remain independent, and no significant lattice deformation occurs [24].

For both twisted graphene and graphene/hBN bilayer heterostructures, Moiré patterns can provide two essential ingredients-topological bands and strong correlations, which are necessary for engineering intrinsic quantum anomalous Hall effects. Such patterns generically produce bands with finite Chern number [25–28], with time reversal symmetry of the single particle band structure enforced by the cancellation of Chern numbers in opposite graphene valleys. Serlin et al. [29] studied intrinsic quantized anomalous Hall effect in a moiré heterostructures. Hey showed that the quantum anomalous Hall (QAH) effect combines topology and magnetism to produce precisely quantized Hall resistance at zero magnetic field. Their observations revealed that the QAH effect is driven by intrinsic strong interactions, which polarize the electrons into a single spin and valley resolved moiré miniband with Chern number \( C = 1 \) [29]. Sharpe et al. [30] and Chen et al. [31] reported time-reversal symmetry breaking in tBLG [30] and graphene/hBN heterostructures [31] at commensurate filling, respectively. These systems show large anomalous Hall effects highly suggestive of an incipient Chern insulator at zero magnetic field (\( B = 0 \)).

In this research, we implement the tight-binding (TB) approaches for twisted two GNs with both rectangular and circular shapes. Our main results show that the circular twisted graphene nanoribbons (tGNs) for small \( \theta \)s are metallic and for large \( \theta \)s are semiconductor, while circular tGNs for both small and large \( \theta \)s exhibit metallic behavior. Moreover, the behavior of electron transport and conductance of these two tGNs for small and large \( \theta \)s manifest Klein paradox in different transport mechanism. We understand that the electronic properties as well as transport process based on the Landauer formalism of tGNs depend on the structural geometry.

2. Model description:

We focus on nanoribbons with atomically precise edges, called zigzag and armchair edges. We consider both rectangular and circular tGN and thG/BNN structures with small \( \theta \)s of (\( \theta = 0.48^\circ \), \( 0.72^\circ \), \( 0.92^\circ \), \( 1.1^\circ \), \( 1.33^\circ \)) and large angles (\( \theta = 3.5^\circ \), \( 6.4^\circ \), \( 9.6^\circ \), \( 13^\circ \)).
and BN relaxation, G-relaxation only and with no relaxation. In-plane lattice relaxation leads to sizeable band gaps in the limit of long moire period. The explicit calculations reported on in this paper are for \( \theta / \alpha = 0, \) the orientation that leads to large experimental gaps. The relevance of this "smoothing" for experiment is discussed. It is demonstrated that this sensitivity of the gap to small distance makes it difficult to predict the gap value for real samples, and because of large barriers and weak thermodynamic drivers these two macroscopic variables are not in practice nonsignificant. In the tight-binding (TB) transport model for (a) circular and (b) rectangular nanoribbons. (c) Symmetry broken and LDOS of Moiré pattern of two graphene nanoribbons for two regimes of \( 0^\circ < \theta < 2^\circ \) and \( 21^\circ < \theta < 30^\circ \) (d) Brillouin zone (BZ) of two rotated graphene layers. (e) Tight-binding (TB) parameters for the twisted model.

21.79°, 27.79°) as shown in Fig. 1, Fig. 2 and Fig. 3, respectively. We Choose these special angles due to the fact that the properties of zigzag tGN under these angles have experimentally been investigated [1,32-36]. We use the TB-Hamiltonian to compute the electronic properties and electron transport of the tGN channels as a function of the twisting angle. Afterwards, we model our system as a finite scattering element or channel, which is connected to two infinite graphene bilayer leads as periodic electrodes. Our target for electron transport of tGNs is applying the Landauer formalism to our system, since the left and right leads, corresponding to the contacts of quantum transport experimental set up, behave as waveguides for transmitting the plane waves into and out of channel as a scattering region.

As starting point, we calculate the electronic properties of zigzag tGNs such as total density of states (DOS) and electronic band structure in the TB-Hamiltonian framework. We construct a low-energy continuum model Hamiltonian that consists of three terms: two TB-Hamiltonian terms for single-layers, which account for the isolated graphene sheets, and one tunneling term that describes hopping between the layers.
Fig. 2: (a) Moiré pattern generated by rotation of two circular zigzag graphene nanoribbons by $\theta = 1.1^\circ$. (b) Spatial local density of states of zigzag tGNs at magic angle $\theta = 1.1^\circ$ and (c) LDOS for small twist-angle ($\theta = 0.48^\circ$, $0.72^\circ$, $0.97^\circ$, $1.1^\circ$, $1.33^\circ$) and (d) band structure of circular zigzag tGNs for magic angle $\theta = 1.1^\circ$. (e) Moiré pattern of two circular graphene nanoribbons by $\theta = 13^\circ$. (f) Spatial local density of states of zigzag tGNs at $\theta = 13^\circ$ and (g) LDOS for large twist-angle ($\theta = 3.5^\circ$, $6.4^\circ$, $9.6^\circ$, $13^\circ$, $21.79^\circ$, $27.79^\circ$) and (h) band structure of circular zigzag tGNs for $\theta = 13^\circ$.

For developing the TB-Hamiltonian for tGN, we first consider two sublattices in each graphene layer, $A_1$, $B_1$ in layer 1, and $A_2$, $B_2$ in layer 2, as presented in Fig. 1. By rotating two graphene nanoribbons by angle $\theta$, tGNs is created, as can be seen in Fig. 1; $t$ is the in-plane hopping of nearest-neighbor, and $\gamma_1$, $\gamma_3$, and $\gamma_4$ are out of plane hopping of the AB-stacked nanoribbons (more details in Ref. [37]). Additionally, $t'(r; r')$ is the interlayer hopping amplitude between sites in the position $r$ and $r'$. By considering this circumstance, we can write down the invariant translational the TB-Hamiltonian with respect to the vector $R_{1,2}$ [37]:

$$H = -t \sum_{ij,\sigma} (b_{iA\sigma}^+ b_{jB\sigma} + \text{H.c.}) + \sum_{\alpha,\beta,\sigma} t'(r_{\alpha}, r'_{\beta}) (b_{\alpha\sigma}^+ b_{\beta\sigma} + \text{H.c.})$$

(1)
where in-plane hopping amplitude is \( t = 2.57 \text{eV} \) and interlayer hopping \( t'(r, r') \) is for position \( r = R_1 + r_s \) and \( r' = R_2 + r_m \). \( b^+ \) and \( b \) are the creation and annihilation operators of an electron with the spin sigma in the top and bottom layers \( s = 1, 2 \) on both sublattices \( \alpha = A, B \) in the supercell [37]. The Fourier transform of the TB-Hamiltonian described in Eq. 1 becomes [37]:

\[
H = \sum_{k, \sigma} t^\pm_k(k) \left( b^+_{sk\alpha} b_{sk\beta} + H. c. \right) + \sum_{\alpha, \beta, k, \sigma} t'(k_\alpha, k'_\beta) \left( b^+_{k_\alpha \sigma} b_{k_\beta \alpha} + H. c. \right)
\]

(2)

where \( b_{sk\sigma} = \frac{1}{N_{sc}} \sum_k e^{-i k r_k} b_{sk\sigma} \) and \( N_{sc} \) is the number of supercells in the bilayer [37]. To calculate the interlayer hopping amplitude i.e. \( t'(r, r') \), we apply the proposed approach in Ref. [38], which take into account the position of neighboring atoms by screening function. At final step, we introduce the \( H = \sum_k \psi_k^i \bar{H} \psi_k \) and N-component operator as [37]:

\[
\bar{H}_K = \begin{pmatrix}
\psi_k = \{b^+_1 A b^+_1 B b^+_2 A b^+_2 B\} \\
0 & \tilde{t}_k^1 & \tilde{t}_k^{11} & \tilde{t}_k^{12} \\
\tilde{t}_k^{1+} & 0 & \tilde{t}_k^{21} & \tilde{t}_k^{22} \\
\tilde{t}_k^{11+} & \tilde{t}_k^{21+} & 0 & \tilde{t}_k^{22+} \\
\tilde{t}_k^{12+} & \tilde{t}_k^{22+} & \tilde{t}_k^{2+} & 0
\end{pmatrix}
\]

(3)

(4)

\[\bar{H} = \begin{pmatrix}
\ldots & V_L & \ldots & \ldots & \ldots \\
V^*_L & H_L & V_L & \ldots & \ldots \\
\ldots & V^*_L & H_L & V_{L,S} & \ldots \\
\ldots & \ldots & V^*_L & H_S & \ldots
\end{pmatrix}
\]

(5)

3. Scattering theory:

To investigate the electron transport in tGNs, we use the wave function framework of the scattering system, which is mathematically equivalent to the non-equilibrium Greens function (NGF) formalism due to Fisher-Lee relation [34]. We modeled the electron transport as two leads (L) connected to scattering region (S) or channel (Figs. 4a and 5a) by the tridiagonal block Hamiltonian as [39]:

\[
\phi_n^i = (\lambda_n)^j \chi_n
\]

(6)

where \( \lambda_n \) is the n-th eigenvalue and \( \chi_n \) is the n-th eigenvector and this wave function obeys the Schrödinger equation [39]:

\[
(H_L + V_L \lambda_n^{-1} + V_{L,S} \lambda_n) \chi_n = E \lambda_n,
\]

(7)

The normalizability of the wave function requires the \( |\lambda_n| \leq 1 \). \( |\lambda_n| < 1 \) gives the evanescent modes, while the \( \lambda_n = 1 \) is the propagating longitudinal channel modes with momentum \( k_n \) as \( \lambda = e^{ik_n} \). The normalized propagating modes are acquired by the expectation value of the particle current \( < I > [39]:

\[
< I > \equiv 2 |\text{Im} \phi_n(j) | V_L |\phi_n(j - 1)| \geq \pm 1
\]

(8)

The propagated modes are incoming waves \( \phi_{in}^n \) waves, outgoing waves \( \phi_{out}^n \) and evanescent waves \( \phi_{ev}^n \). The scattering states in the leads become [39]:

\[
\psi_n(i) = \phi_{in}^n(i) + \sum_m S_{mn} \phi_{out}^n(i) + \sum_m \tilde{S}_{pm} \phi_{ev}^n(i),
\]

(9)
Fig. 3: (a) Moiré pattern generated by rotation of two rectangular zigzag graphene nanoribbons by magic angle $\theta = 1.1^\circ$. (b) Spatial local density of states of zigzag tGNs at magic angle $\theta = 1.1^\circ$ and (c) LDOS for small twist-angle ($\theta = 0.48^\circ, 0.72^\circ, 0.97^\circ, 1.1^\circ, 1.33^\circ$) and (d) band structure of rectangular zigzag tGNs for magic angle $\theta = 1.1^\circ$. (e) Moiré pattern of two rectangular zigzag graphene nanoribbons by $\theta = 13^\circ$. (f) Spatial local density of states of zigzag tGNs at $\theta = 13^\circ$ and (g) LDOS for large twist-angle ($\theta = 3.5^\circ, 6.4^\circ, 9.6^\circ, 13^\circ, 21.79^\circ, 27.79^\circ$) and (h) band structure of rectangular tGNs for $\theta = 13^\circ$. (i) Variation of bandgap versus tAs, which shows metallic behavior for $\theta \leq 1.1^\circ$ and semiconductor for $\theta > 1.1^\circ$.

where $S_{nm}$ is the scattering matrix and the scattering wave function for whole of the system is:

$$\psi_n(0) = \Phi_n^S$$  \hspace{1cm} (10)

To calculate the conductance ($\sigma_{ab}$) of channel connected to two left and right electrodes (a, b), the differential conductance $G_{ab} = dI/I/dV_S$ is extracted from Landauer equation [39]:
Fig. 4: (a) Circular channel-electron transport of zigzag tGNs at magic angle $\theta = 1.1^\circ$. (b) Electron transmission (T(E)) of circular zigzag tGNs for small $\theta < 2^\circ$ ($\theta = 0.48^\circ, 0.97^\circ, 1.33^\circ$). (c) Density plot of conductance ($\sigma(E)$) vs circular channel. (d) Circular channel-electron transport of zigzag tGNs at $\theta = 13^\circ$. (e) T(E) of circular zigzag tGNs for large $\theta > 2^\circ$ ($\theta = 3.5^\circ, 13^\circ, 27.79^\circ$). (f) Contour plot of $\sigma(E)$ vs circular channel.

The LDOS or current density can be calculated by $\phi_n$ [39]:

$$< c_i^+ c_j > = \int \frac{dE}{2\pi} \sum_n f_n(E) \phi_n^<(j) [\phi_n^<(j)]^*,$$

where $f_n(E)$ is the Fermi function of the leads connected to channel $n$; $f_n(E) = \frac{1}{1 + e^{E - \mu_n/k_B T_n}}$. In this step, we impose a perpendicular uniform magnetic field to the circular and rectangular tGNs; $B = (0, 0, B)$, which we neglect spin Zeeman splitting for simplicity. $\phi$ is the number of magnetic fluxes per a unit cell ($\phi = BA$), which is measured in units of the quantum flux $\phi_0 = h/e$ [40]. The TB-Hamiltonian in the magnetic field has no translational symmetric due to the spatial
dependence of the vector potential. Taking into consideration the magnetic field to the TB-Hamiltonian will add a phase factor \( (\phi_{ij}) \) to the transfer integral as [40]:

\[
H_{TB} = -\sum_{i,j} t(R_i,R_j) e^{i\phi_{ij}} |\psi_i \rangle \langle \psi_j | + H.c. \tag{13}
\]

\[
\phi_{ij} = -\frac{e}{\hbar} \int_{R_j} A(r). dr \tag{14}
\]

finite temperature is based upon the Kubo-Bastin formula [41]. The linear response theory gives the Kubo formula for calculating the conductivity tensor. The static conductivity in the limit \( \omega \rightarrow 0 \), which is known as the Kubo-Bastin formula, is [41]:

\[
\sigma_{\alpha\beta}(\mu,T) = \frac{i e^2 \hbar}{\alpha} \int_{-\infty}^{\infty} \delta(\varepsilon - H) \frac{d\varepsilon}{d\varepsilon} f(\varepsilon)
\]

\[
\text{where } \Omega \text{ is the volume, } v_\alpha \text{ and } v_\beta \text{ are the } \alpha \text{ and } \beta \text{ components of the velocity operator, } G^* \text{ and } G \text{ are the advanced and retarded Green’s functions, respectively, and } f(\varepsilon) \text{ is the Fermi-Dirac distribution for a chemical potential } \mu \text{ and temperature } T \text{ [41].}
\]

polynomials, in which the kernel polynomial are implemented [42,43], as a scalable and efficient way [41,44-46]. First, we rescale the TB-Hamiltonian as \( \tilde{H} \) with the energy spectrum of upper \( E^* \) bound mapped to +1, and lower \( E \) bound mapped to -1. Then, the rescaled TB-Hamiltonian is written by \( \tilde{H} \) and rescaled energy \( \tilde{\varepsilon} \) as [41]:

\[
\delta(\varepsilon - H) = \frac{2}{\pi \sqrt{1 - \tilde{\varepsilon}^2}} \sum_{m=0}^{M} \delta_{m,0 + 1} T_m(\tilde{H}) \tag{16}
\]

\[
G^\pm(\varepsilon, H) = \mp \frac{2i}{\sqrt{1 - \tilde{\varepsilon}^2}} \sum_{m=0}^{M} \delta_{m,0 + 1} T_m(\tilde{H}) \tag{17}
\]

where \( T_m(x) \) is the first kind and order \( m \) of the Chebyshev polynomial and defined as: \( T_m(x) = \cos [m \arccos(x)] \). By substituting the \( T_m(x) \) in Eq. 15, we acquire [41]:

\[
\sigma_{\alpha\beta}(\mu,T) = \frac{4e^2 \hbar}{\pi \Omega \Delta E^2} \int_{-\infty}^{\infty} d\varepsilon \frac{f(\varepsilon)}{(1 - \varepsilon^2)^2} \sum_{n,m} \Gamma_{nm}(\varepsilon) H_{nm} \tag{18}
\]

4. Results and discussions:
In this work, we have considered circular and rectangular zigzag tGNRs, as presented in Fig. 1, Fig. 2 and Fig. 3, respectively. As starting point of studying the electronic properties of tGNs, spatial local density of states (LDOS) for two regimes of \( \theta < 2^\circ \) and \( \theta > 2^\circ \) is computed by the TB-Hamiltonian. The calculated LDOS of zigzag tGNs of two layers in Moiré pattern is a function of energy and position (E, r), where the interlayer hopping terms took into account in the TB Hamiltonian and LDOS can be computed by [47]:

\[
\rho(E, \vec{r}) = < \vec{r} | \delta(E - H) | \vec{r} > \tag{19}
\]

Here we calculate the energy spectrum of diagonal and off-diagonal conductivity for any carbon as a function of position \( \vec{r} \), as can be seen in Fig. 2b and Fig. 2f for small and large circular tGNs, respectively; and in Fig 3b and Fig. 3f for small and large rectangular tGNs, respectively. Moreover, in our model for \( \theta = 0^\circ \), the bilayer GN is an AB stacked structure and then for large angles AA region grows with enhanced localized states. As shown by the theoretical [48-50] and experimental [51,52] studies of tBLG, the ±E of Van-Hove singularities of density of states increases linearly with the tAs \( \theta \sim > 2^\circ \). We consider LDOS since LDOS is commensurate with experimental data acquired by scanning tunneling microscopy (STM) images. Fig. 2c, Fig. 2g Fig. 3c, and Fig. 3g present the LDOS of all systems, which are in good agreement with STM observation of Ref. [3].
**Fig. 5:** (a) Rectangular channel-electron transport of zigzag tGNs at magic angle \( \theta = 1.1^\circ \). (b) Electron transmission (T(E)) of rectangular zigzag tGNs for small \( \theta < 2^\circ \) (\( \theta = 0.48^\circ, 0.97^\circ, 1.33^\circ \)). (c) Density plot of conductance (\( \sigma(E) \)) vs rectangular channel. (d) Rectangular channel-electron transport of zigzag tGNs at \( \theta = 13^\circ \). (e) T(E) of circular zigzag tGNs for large \( \theta > 2^\circ \) (\( \theta = 3.5^\circ, 13^\circ, 27.79^\circ \)). (f) Contour plot of \( \sigma(E) \) vs rectangular channel.

In the second step, we calculated the electronic band structure of tGNs and plotted in **Fig. 2d** and **Fig. 2h** for circular tGNs with small and large tAs, respectively, while **Fig. 3d** and **Fig. 3h** show the band structure of rectangular tGNs. Analysis of these figures reveals that the band structure depends on the shape of tGNs, which can change the bandgap energy (\( E_g \)) as presented in **Table 1** and **Fig. 3i**. The reported data in **Table 1** reveals that the circular tGNs are metal for different tAs, while the rectangular one is metal for small angles and semiconductor for larger angles. It’s worth noting that the band structures for small angles of rectangular tGNs are in close agreement with the band structures of AB bilayer GNs reported in Ref. [37]. Interestingly, **Fig. 3d** and **Fig. 3h** indicate two flat bands near the Fermi level, which prove the local electron states created by Moiré pattern in the circular tGNs.

**Table 1. Bandgap energy \( (E_g) \) of circular and rectangular tGNs for different tAs (\( \theta \)).**

| \( \theta \) (degree) | 0.48 | 0.72 | 1.1 | 1.33 | 1.5 | 2 | 6.4 | 9.6 | 13 | 17 | 21.79 | 27.79 |
|----------------------|------|------|-----|------|-----|---|-----|-----|----|----|--------|--------|
| \( E_g \) (meV)      |      |      |     |      |     |   |     |     |    |    |        |        |
| Circular             | 0    | 0    | 0   | 0    | 0   | 0 | 0   | 0   | 0  | 0  | 0      | 0      |
| Rectangular          | 0    | 0    | 0   | 90   | 96  | 26| 7   | 2   | 7  | 10 | 12     | 14     |

The valence bands (VBs) near Fermi level for \( \theta = 13^\circ \) (**Fig. 3h**) are flatter than the VB for magic angle \( \theta = 1.1^\circ \) (**Fig. 3d**), which confirms more local electron states for large tAs and supports the LDOS data. Moreover, multi-flat bands shown in **Fig. 3d** and **Fig. 3h** prove that the local
electron states of rectangular tGNs, which fourfold degenerate flat bands of $\theta = 13^\circ$ (Fig. 3h), are sign of enhanced local electron states compared to twofold degenerate flat bands of magic angle $\theta = 1.1^\circ$ (Fig. 3d) that supports our previous results of LDOS (Fig. 3b and Fig. 3f).

**Fig. 6:** Quantum Hall effect of circular tGNs with rotation angles of (a) magic angle $\theta = 1.1^\circ$, (b) $\theta = 9.6^\circ$ and (c) $\theta = 21.79^\circ$. Top panels display the Hall conductivity $\sigma_x$ and $\sigma_y$ and Hall effect quantized spectrum as functions of magnetic field, where the bottom panels show the LDOS of tGNs at magnetic field ($B = 40$ T). The quantized values of Hall conductivity are separated by different colors.

In this step, we calculate the transmission ($T(E)$) and conductivity ($\sigma(E)$) of circular/rectangular tGN channels connected two GN leads, as shown in **Fig. 4a** and **Fig. 5a**, by applying the wave function of the TB-Hamiltonian formalism as described in **Eq. 11**. The transmission and conductance of circular nanochannels as a function of barrier heights is depicted in **Fig. 4** for different tAs at electron energy of 250 meV. The analysis of **Fig. 4b** and **Fig. 4e** confirms that the Klein paradox for $T(E)$ and $\sigma(E)$ of circular channels at both small and large tAs. $T(E)$ show that electron can transport by any potential barrier without confinement effect. Moreover, to investigate the structural geometry dependent of transmission and conductance, we compute $T(E)$ and $\sigma(E)$ of rectangular tGNs (**Fig. 5**). Interestingly, the transmission behavior of circular and rectangular tGNs drastically differs. The transmission of rectangular tGN channels with large $\theta > 2^\circ$ is close to bilayer graphene, while the transmission for small $\theta < 2^\circ$ indicates more fluctuation with smaller magnitude than larger tAs. The large magnitude of $T(E)$ in **Fig. 5e** and **Fig. 5f** can be associated into the enhanced charge carriers which causes localized electron states and decoupled GN layers. While, in small tAs fluctuation in $T(E)$ and $\sigma(E)$ proves more electronic states are coupled on both layers and less charge carrier can transport, which is in a good agreement with the previous study presented in Ref. [47].
circular thG/BNNs for symmetric peaks near the Fermi energy, which is \( \theta = 3.5^\circ \), generated by rotation of circular graphene nanoribbon on circular BN nanoribbon by \( \theta = 1.1^\circ \). Fig. 7 presents several Landau levels around Fermi energy. The quantized values of Hall conductivity are separated by different colors.

**Hall effect:** We compute and show the longitudinal (\( \sigma_{xx} \)) and off-diagonal (\( \sigma_{xy} \)) Hall conductivities and quantum Hall quantized spectrum as function of magnetic field for both circular and rectangular tGNs for magic angle \( \theta = 1.1^\circ \) and larger tAs \( \theta = 9.6^\circ \), 21.79°, as demonstrated in Fig. 6 and Fig. 7, respectively. These quantized Hall conductivity spectrum of circular tGNs (Fig. 6) reveals several quantized Landau level, similar to graphene monolayer. However, rectangular tGNs spectrum in Fig. 7 exhibits the continuity of Hall conductivity and complex behavior. The off-diagonal Hall conductivity of Circular tGNs; \( \sigma_{xy} \), shows the hole-like Landau levels around Fermi energy. We plot the LDOS for both circular and rectangular tGNs under an applied magnetic field with the strength of \( B = 40T \) in bottom panels of Fig. 6 and Fig. 7, respectively. The LDOS in Fig. 6 presents several Landau levels with zero density of electron states close to the Dirac point, while Fig. 7 for rectangular tGNs indicates the non-zero electron states at Dirac point, confirming metal behavior of circular tGNs under the applied magnetic field.

**Twisted heterostructure of G/BN nanoribbons (thG/BNNs):** The Moiré pattern in Fig. 8 generated by rotation of circular graphene nanoribbon on circular BN nanoribbon by \( \theta = 1.1^\circ \) and 13°, which create the twisted heterostructure of G/BN nanoribbons (thG/BNNs). The LDOS of circular thG/BNNs for small twist-angle \( (\theta = 0.48^\circ, 0.72^\circ, 0.97^\circ, 1.1^\circ, 1.33^\circ) \) and large twist-angle \( (\theta = 3.5^\circ, 6.4^\circ, 9.6^\circ, 13^\circ, 21.79^\circ, 27.79^\circ) \) are computed and plotted in Fig. 8. The LDOS shows the symmetric peaks near the Fermi energy, which is confirmed by flat bands at the band structure of circular thG/BNNs for
Fig. 8: (a) Moiré pattern generated by rotation of circular graphene nanoribbon on the circular BN nanoribbons by $\theta = 1.1^\circ$. (b) LDOS for small twist-angle ($\theta = 0.48^\circ, 0.72^\circ, 0.97^\circ, 1.1^\circ, 1.33^\circ$) and (c) band structure of circular thG/BNNs for $\theta = 1.1^\circ$. (d) Moiré pattern of circular thG/BNNs by $\theta = 13^\circ$. (e) LDOS for large twist-angle ($\theta = 3.5^\circ, 6.4^\circ, 9.6^\circ, 13^\circ, 21.79^\circ, 27.79^\circ$) and (f) band structure of circular thG/BNNs for $\theta = 13^\circ$.

Fig. 9: (a) Moiré pattern generated by rotation of rectangular zigzag graphene nanoribbon on rectangular zigzag BN nanoribbon by $\theta = 1.1^\circ$. (b) LDOS for small twist-angle ($\theta = 0.48^\circ, 0.72^\circ, 0.97^\circ, 1.1^\circ, 1.33^\circ$) and (c) band structure of rectangular thG/BNNs for magic angle $\theta = 1.1^\circ$. (d) Moiré pattern of the rectangular zigzag thG/BNNs by $\theta = 13^\circ$. (e) LDOS for large twist-angle ($\theta = 3.5^\circ, 6.4^\circ, 9.6^\circ, 13^\circ, 21.79^\circ, 27.79^\circ$) and (f) band structure of rectangular thG/BNNs for $\theta = 13^\circ$. 
Fig. 10: (a) Circular channel-electron transport of thG/BNNs at magic angle $\theta = 1.1^\circ$. (b) Electron transmission ($T(E)$) of circular thG/BNNs for small $\theta < 2^\circ$ ($\theta = 0.48^\circ, 0.97^\circ, 1.33^\circ$). (c) Circular channel-electron transport of tGNs at $\theta = 13^\circ$. (d) $T(E)$ of circular tGNs for large $\theta > 2^\circ$ ($\theta = 3.5^\circ, 13^\circ, 27.79^\circ$). (e) Density plot of conductance ($\sigma(E)$) vs circular channel.

Fig. 11: (a) Rectangular channel-electron transport of thG/BNNs at magic angle $\theta = 1.1^\circ$. (b) Electron transmission ($T(E)$) of rectangular thG/BNNs for small $\theta < 2^\circ$ ($\theta = 0.48^\circ, 0.97^\circ, 1.33^\circ$). (c) Circular channel-electron transport of tGNs at $\theta = 13^\circ$. (d) $T(E)$ of rectangular tGNs for large $\theta > 2^\circ$ ($\theta = 3.5^\circ, 13^\circ, 27.79^\circ$). (e) Density plot of conductance ($\sigma(E)$) vs rectangular channel.
levels of magnetic field, we realize that the quantized electron states result in the quantized Landau spectrum as function of magnetic field for both circular and rectangular heterostructures. Fig. 9 shows the Moiré pattern generated by rotation of rectangular zigzag graphene nanoribbon on rectangular zigzag BN nanoribbon by \( \theta = 1.1^\circ \) and \( 13^\circ \). The LDOS of rectangular thG/BNNs for small and large twist-angle are shown in Fig. 9b, and Fig. 9e. The LDOS shows the several localized electron states near and on the Fermi energy, which is confirmed by flat bands at the band structure of \( \theta = 1.1^\circ \) and \( 13^\circ \) in this Figure. Also, near the Fermi energy there is two flat bands separated by 0.1 eV and 0.05 eV for \( \theta = 1.1^\circ \) and \( 13^\circ \) respectively. Therefore, the rectangular thG/BNNs shows the semiconductor behavior with zero group velocity and low mobility for electron carriers on the Fermi energy. We conclude that the electron transmission and conductance of rectangular zigzag thG/BNNs will be low due to low mobility of electron carriers. By calculating transmission function and plotting on Fig. 10, and Fig. 11 we notice that the transmission of these heterostructure is 7 orders of magnitude less than tGNs, supporting our electronic properties of heterostructures.

**Hall effect of heterostructures:** To investigate the hall effect of circular heterostructures, we calculated the longitudinal (\( \sigma_{xx} \)) and off-diagonal (\( \sigma_{xy} \)) Hall conductivities and quantum Hall quantized spectrum as function of magnetic field for both circular (Fig. 12) and rectangular (Fig. 13) thG/BNNs for \( \theta = 1.1^\circ \) and larger tAs \( \theta = 9.6^\circ \), 21.79. By considering LDOS in the presence of magnetic field, we realize that the quantized electron states result in the quantized band levels of \( \sigma_{xx} \) and \( \sigma_{xy} \). For rectangular heterostructures in the presence of magnetic fields, LDOS

![Fig. 12: Quantum Hall effect of circular thG/BNNs with rotation angles of (a) magic angle \( \theta = 1.1^\circ \), (b) \( \theta = 9.6^\circ \) and (c) \( \theta = 21.79^\circ \). Top panels display the Hall conductivity \( \sigma_{xx} \) and \( \sigma_{xy} \) and Hall effect spectrum as functions of magnetic field, where the bottom panels show the LDOS of thG/BNNs at magnetic field (B = 40 T). The quantized values of Hall conductivity are separated by different colors.](image)
shows multiple localized states without symmetry near the Fermi energy, which creates complex behavior of $\sigma_{xx}$ (by gap states) and $\sigma_{xy}$.

\( \text{(a) Rectangular thG/BN} \)  \( \theta = 1.1^\circ \)  \( \text{(b) Rectangular thG/BN} \)  \( \theta = 9.6^\circ \)  \( \text{(c) Rectangular thG/BN} \)  \( \theta = 21.79^\circ \)

Fig. 13: Quantum Hall effect of rectangular thG/BNNs with rotation angles of (a) $\theta = 1.1^\circ$, (b) $\theta = 9.6^\circ$ and (c) $\theta = 21.79^\circ$. Top panels display the Hall conductivity $\sigma_{xx}$ and $\sigma_{xy}$ and Hall effect spectrum as functions of magnetic field, where the bottom panels show the LDOS of thG/BNNs at magnetic field ($B = 40$ T). The quantized values of Hall conductivity are separated by different colors.

**Armchair tGNs:** Nanoribbons with different edge termination rise to different electronic properties with localized edge states. For instance, geometrical control of edge of GNs converts it to metal or semiconductor. To investigate the effect of structural geometry on the electronic and electron transport of twisted structures, the electronic bandstructure of circular and rectangular armchair GNs for magic angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$ are calculated and shown in Fig. 14, and Fig. 15. The bandstructure of these structures reveal that the armchair circular tGNs behave as semimetal materials and is gapless with Dirac cone at Fermi energy. However, the armchair rectangular tGNs are semiconductor with band gap of 0.24 eV and 0.12 eV for twisted angle of $\theta = 1.1^\circ$ and $\theta = 13^\circ$ respectively. The transmission function of the armchair circular and rectangular of tGNs for $\theta = 1.1^\circ$, $13^\circ$, $21.79^\circ$ are shown in Fig. 16, and Fig. 17. Figure 17 LDOS for armchair rectangular tGNs for energy range [-0.5...0.5] eV for large twisted angle are in good agreement with result of reference [53]. For instance, LDOS in Fig. 17 at zero energy for various twisted angle is not zero, which is consistent with LDOS of figure 5.6 in the reference [53].

**Armchair thG/BNNs:** For armchair of heterostructures, the electronic bandstructure of armchair circular and rectangular thG/BNNs for two angles $\theta = 1.1^\circ$ and $\theta = 13^\circ$ are indicated in Fig. 18, and Fig. 19. The armchair of twisted circular heterostructures behave as metal, however, the rectangular armchair of heterostructures is semiconductor with band gap of 0.13 eV and 0.08 eV for twisted angle of $\theta = 1.1^\circ$ and $13^\circ$ respectively.
Fig. 14: Moiré pattern generated by rotation of two armchair circular graphene nanoribbons by magic angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$. Band structure of armchair circular tGNs for magic angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$.

Fig. 15: Moiré pattern generated by rotation of two armchair rectangular graphene nanoribbons by magic angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$. Band structure of armchair rectangular tGNs for magic angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$. 
Fig. 16: LDOS (a-c) and electron transmission (d-f) of armchair circular tGNs at magic angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$ and $\theta = 21.79^\circ$.

Armchair Rectangular tGNs

Fig. 17: LDOS (a-c) and electron transmission (d-f) of armchair rectangular tGNs at magic angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$ and $\theta = 21.79^\circ$. 
**Fig. 18:** Band structure of twisted heterostructure of armchair circular thG/BNNs for twisted angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$.

**Fig. 19:** Band structure of twisted heterostructure of armchair rectangular thG/BNNs for twisted angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$. 
It’s worth noting that the band gap opening for armchair is greater than zigzag rectangular heterostructures (Fig. 9). The transmission function and LDOS of these armchair circular and rectangular heterostructures for $\theta = 1.1^\circ$, $13^\circ$, $21.79^\circ$ are shown in Fig. 20, and Fig. 21. The quantum transport of metallic circular armchair of heterostructure dominates relative to semiconductor armchair rectangular thG/BNNs.

**Conclusions:**
The transmission, conductance and Hall effect of circular and rectangular tGN and thG/BNN channels are modeled and computed by applying the TB-Hamiltonian. Moiré pattern of tGNs with different twist-angles creates new electron states and tunes the electron transport. The electronic band structure reveals the phase transition of rectangular tGNs from metallic for small angles to semiconductor for large angles, while circular one is metallic for two regimes of small and large angles. Multi-flat bands and degenerate valance bands observed for two tGNs are the signature of local density of states with zero Fermi velocity and electron decoupling of GNS.

**Fig. 20:** LDOS (a-c) and electron transmission (d-f) of twisted heterostructure of armchair circular thG/BNNs at angle $\theta = 1.1^\circ$ and $\theta = 13^\circ$ and $\theta = 21.79^\circ$. 
Our findings highlight the Klein paradox-transport of relativistic carrier through wide potential barrier- in circular tGN channels. Moreover, the calculated Hall conductivity spectrum for wide range of magnetic field exhibits different behavior for circular and rectangular tGNs. For instance, the circular tGNs reveal quantized hall conductivity, while rectangular one shows the continuity of Hall conductivity. We extend our study to the quantum transport and Hall effect of twisted heterostructures of G/BNNs. The rectangular thG/BNNs shows the semiconductor behavior, while the circular one is metal. The electron transmission and conductance of circular thG/BNNs dominate regard to the rectangular heterostructures with low mobility of electron carriers. We conclude that the geometry control of nanoribbons affects transport properties due to creation of localized edge states. For instance, zigzag nanoribbons with enhanced localized electron states dominate their electron transport. Collectively, our findings suggest that by manipulating tAs in tGNs and thG/BNNs, we can create nano-transistors, which can be used in the electronic devices.

**Conflict of interest:**

The authors declare that there is no conflict of interest.
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