Spin–orbit proximity effect and topological superconductivity in graphene/transition-metal dichalcogenide nanoribbons

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Abstract
Spin–orbit coupling (SOC) plays a determinate role in spintronics and topological physics. Previous studies indicate that the SOC in graphene nanoribbon (GNR) can be enhanced by the proximity effect from two-dimensional transition-metal dichalcogenide (2D-TMD). However, the bulk inversion symmetry of GNR/2D-TMD restricts further increase of the proximity-induced SOC in GNR. In this view, we introduce a TMD nanoribbon (TMDNR) with finite width, and propose three methods to break the bulk inversion symmetry, i.e. defects in TMDNR, spatial interlayer edge coupling, and twist between GNR and TMDNR, which can further enhance the SOC in the GNR by roughly 30 times, 20 times and 150 times, respectively, depending on the relative energy between the Dirac point of GNR and the states of TMDNR. Furthermore, the significantly enhanced SOC can drive the GNR into a topological superconducting phase. By introducing the Zeeman splitting and s-wave superconductivity in the GNR, quasi one-dimensional topological superconductivity and Majorana zero modes (MZMs) can be achieved in the GNR. At last we propose a feasible experimental method to realize and manipulate MZMs in the GNR/TMDNR system.

1. Introduction
Graphene is a fascinating material which exhibits outstanding electrical transport properties and presents great application prospects in nanoelectronics [1]. However, the weak intrinsic spin–orbit coupling (SOC), only about 10 μeV in pristine graphene [2, 3], hinders the control and tunability of possible spintronic devices [4]. The recent experiments have proved that the spin–orbit splitting in graphene can be strongly enhanced by proximity to the TMD substrates [5–10]. The giant SOC originates from a modification of graphene band structure [6], and can be controlled by a gate voltage [6, 7, 11]. The theoretical studies on van der Waals heterostructures formed by graphene and TMD have shown that the proximity-induced SOC is composed of the valley Zeeman and Rashba type terms [12–15], and that such SOC can also be tuned by varying the twist angle between the TMD and graphene [15–17]. Moreover, the enhanced SOC induced in graphene by a TMDC could enable phenomena such as pseudohelical edge states [18], the quantum spin Hall state [19, 20], the quantum anomalous Hall effect [21, 22] and topological superconductivity [23, 24].

Recently, the proximity-induced SOC in graphene nanoribbon (GNR) has attracted great attention due to the realization of the quasi-1D topological superconductor [23–25]. Compared to the 2D graphene/TMD
stacking, the spin–orbit proximity effect in the GNR is very different, and the induced SOC is more diverse depending on the conductivity of two-dimensional transition-metal dichalcogenide (2D-TMD). The first-principle calculation shows that the proximity-induced spin splitting energy in the GNR can reach 20 to 40 meV when the 2D-TMD is metallic, but is much smaller if the 2D-TMD is semiconducting [25]. However, most 2D-TMDs are semiconducting materials which not only preserve high electronic quality of GNR [26], but also exhibit extremely strong SOC to ensure the efficiency of spin-orbital splitting in graphene [27–30]. Therefore, it is essential to explore effective methods to enhance the SOC in the GNR induced by the proximity effect of semiconducting TMD and understand the potential physics. Especially, the enhanced SOC plays an important role to realize the topological superconductivity in GNRs [23, 24, 31].

In this work, we introduce a TMD nanoribbon (TMDNR) with finite width, and construct different GNR/TMDNR systems to investigate the proximity-induced SOC in the GNR. When a narrow GNR lies in the middle region of a wide TMDNR, the proximity-induced SOC in the GNR is weak. The reason is that the wide TMDNR is approximately considered as a 2D-TMD substrate, and the protected bulk inversion symmetry of GNR/2D-TMD restricts further increase of the proximity-induced SOC in the GNR [25]. By adjusting the relative energy between the Dirac point of the GNR and the bulk states of the TMDNR, the SOC can be enlarged but is still not enough to drive the GNR into the topological superconducting phases. On this account, we propose three methods to break the inversion symmetry and further enhance the induced SOC in the GNR, i.e. adding defects in the TMDNR, spatial interlayer edge coupling, and twist between the GNR and TMDNR. When the GNR is directly coupled with the edge of TMDNR, we find that the edge states play determinant roles in the spin–orbit proximity effect instead of the bulk states of TMDNR. Especially, as the Dirac point of GNR is close to the edge states of TMDNR, the induced SOC in the GNR can be further enhanced by 20 to 150 times comparing to the structure with bulk inversion symmetry case. Based on the enhanced SOC, the topological superconductor is realized and Majorana zero modes (MZMs) are observed at both ends of the GNR when the Zeeman field and s-wave superconductivity are presented in the system. Moreover, by stacking several narrow GNR on a wide TMDNR under topological superconducting phase, multiple MZMs can be generated and even transferred by varying the chemical potential spatially and the non-uniform Zeeman field. The GNRs/TMDNR system provides an alternative platform to realize topological superconductor and generate multiple MZMs.

The rests of the paper are organized as follows. In section 2, the tight-binding model is introduced to describe the spin–orbit proximity effect in GNR/TMDNR structure. In section 3.1, three ways are applied to induce giant SOC in the GNRs. In section 3.2, we present the realization of the topological superconductivity and multiple MZMs in the GNR/TMDNR systems. In section 4, the experimental realization of our system is proposed. In section 5, concluding remarks are given.

2. Tight-binding model

Figure 1(a) shows the schematic graphene/TMD commensurate structure without relative twist, where \( a_G (=2.46\ \text{Å}) \) and \( a_M (=3.075\ \text{Å}) \) are the primitive vectors of graphene and TMD, respectively. Obviously, \( a_G = \frac{3}{4} a_M \) in real space. The 5/4 supercell gives the commensurability, and the enlarged honeycomb lattice contains 50 carbon atoms in the graphene layer, 16 M atoms and 32 X atoms in the TMD layer (MX\(_2\) type). The density functional theory calculations [5, 32–35] and tight-binding formalisms [15, 36] have demonstrated that the 5/4 supercell can give effective description of the electronic property. With the van der Waals correction between graphene and TMD, the optimized interlayer distance is 3.34 Å [7].

In view of the dominant contribution from M atoms to the low energy bands in the TMD, the model Hamiltonian of the graphene/TMD heterostructure is described in terms of two independent constituent subsystems and an interlayer coupling term, i.e. \( H = H_G + H_M + H_T \). \( H_G \) describes the Hamiltonian of graphene in terms of \( \rho \) atomic orbital [1],

\[
H_G = -\mu_G \sum_{i,s} c_{i,s}^\dagger c_{i,s} - t_G \sum_{\langle i,j \rangle,\sigma} c_{j,\sigma}^\dagger c_{i,\sigma} + \text{h.c.,} \tag{1}
\]

where \( c_{i,s}^\dagger (c_{i,s}) \) creates (annihilates) an electron with spin \( s \) at site \( i \), \( \mu_G \) is the chemical potential, and \( t_G \) \((\approx -2.7 \text{ eV})\) is the nearest-neighbors coupling of graphene. In view of the very weak intrinsic SOC in graphene, the relative terms are neglected. \( H_M \) is the Hamiltonian of TMD monolayer [15, 35, 37],

\[
H_M = -\mu_{\text{TMD}} \sum_{i,\gamma,\delta} \alpha_{\gamma,i,\delta}^\dagger \alpha_{\gamma,i,\delta} + \sum_{i,\gamma,\delta} \varepsilon_{\gamma,i} \alpha_{\gamma,i,\delta}^\dagger \beta_{\gamma,i,\delta} + \sum_{\langle i,j \rangle,\gamma,\delta} \tau_{\gamma,\delta,\gamma',\delta'} \alpha_{\gamma,i,\delta}^\dagger \alpha_{\gamma',j,\delta'} + \text{i} \lambda \sum_{i,\gamma,\delta,\gamma'} \sum_{\gamma'' \neq \gamma, \gamma' \neq \gamma''} \alpha_{\gamma,i,\delta}^\dagger \sigma_{\gamma'',\gamma'} \alpha_{\gamma',i,\delta} + \text{h.c.} \tag{2}
\]
\( \alpha_{\gamma \sigma}(\alpha_{p \gamma}) \) creates (annihilates) an electron with orbital \( \gamma \) and spin \( s \) at site \( i \), where \( \gamma \) describes three \( d \) orbitals \((d_{x^2}, d_{y^2}, d_{z^2})\) of the \( M \) atom. \( \epsilon_{\gamma \sigma} \) considers the on-site energy of the \( M \) atom with orbital \( \gamma \) and spin \( \sigma \); \( \mu_{\text{TMD}} \) is the chemical potential of the TMD, which can be tuned by the gate voltage; \( \tau_{i \gamma j \gamma'} \) describes the hopping between orbital \( \gamma \) of the \( i \)th \( M \) atom and orbital \( \gamma' \) of the nearest \( j \)th \( M \) atom (marked as \( \tau_{1-2} \) in figure 1(a)); \( \lambda \) is the SOC parameter, which includes the on-site \( L \cdot S \) term of all the \( M \) atoms [37–39]; \( \sigma_{\alpha\beta} \) is the Pauli matrix in terms of the same spin and different orbitals. The interlayer coupling \( H_T \) between \( p_x \) orbitals of graphene and \( d \) orbitals of the \( M \) atoms in TMD is given by [15, 35, 36]

\[
H_T = \sum_{i \neq j, \gamma, \sigma} t_{ij \gamma \sigma} \exp[-R_{ij} / \eta] \alpha_{ij \gamma \sigma}^\dagger \alpha_{ij \gamma \sigma} + \text{h.c.,}
\]

where \( R_{ij} = |R_{ij}| \) describes the distance between the \( i \)th \( M \) atom and the \( j \)th \( C \) atom, and \( \eta = 5 / \sqrt{3} |a_c| \) is defined to normalize \( R_{ij} \); \( t_{ij \gamma \sigma} \) describes the effective coupling between \( p_x \) orbital of the \( j \)th \( C \) atom and \( \gamma \) orbitals of the \( i \)th \( M \) atom. According to Slater–Koster approach [40], \( t_{ij \gamma \sigma} \) takes the form

\[
\begin{align*}
t_{p_x d_{x^2-y^2}} &= \sqrt{3} n_x (n_x^2 + n_y^2) V_{pdz} - \frac{1}{2} n_x (n_x^2 + n_y^2 - 2n_z^2) V_{pdx}, \\
t_{p_x d_{z^2}} &= \sqrt{\frac{3}{2}} n_x (n_x^2 - n_y^2) V_{pdx} - n_x (n_x^2 - n_y^2) V_{pdd}, \\
t_{p_x d_{x^2-y^2}} &= n_x n_y n_z (\sqrt{3} V_{pdx} - 2 V_{pdd}),
\end{align*}
\]

where \( n_x = R_{ij} / R_{ij} \cdot i, n_y = R_{ij} / R_{ij} \cdot j \) and \( n_z = R_{ij} / R_{ij} \cdot k \). \( V_{pdx} \) and \( V_{pdd} \) are constants that couple the \( p \) orbital and \( d \) orbital through \( \pi \) and \( \delta \) bonds, respectively. In this calculation, we set \( V_{pdx} = -0.232 \) eV and \( V_{pdd} = 0.058 \) eV [15, 36], which do not affect the main conclusions qualitatively. In order to confirm the accuracy of the three-\( d \)-orbital model, a more complicated eleven-orbital model is also implemented, where five \( d \) orbitals of the \( M \) atom \((d_{x^2-y^2}, d_{z^2}, d_{x^2}, d_{x^2+y^2}, d_{x^2-z^2})\) and six \( p \) orbitals of \( X \) atom \((p_x, p_y, p_z, p_{xz}, p_{yz}, p_{zx})\) are considered simultaneously [16, 41]. Numerical results show that the proximity-induced SOC behaviors on the GNR are roughly the same from the three-\( d \)-orbital model and eleven-orbital model. Therefore, we are comfortable to employ the three-\( d \)-orbital model in all the following calculation.

The twisted graphene/TMD structure can be generated by rotating the graphene layer by \(-\varphi/2\) angle and the TMD layer by \(+\varphi/2\) angle [24, 42]. For specific \( \varphi \), a proper Moiré superlattice can be formed with
primitive lattice vectors \( \mathbf{L}_1 \) and \( \mathbf{L}_2 \) on the twisted graphene/TMD. \( \mathbf{L}_1 \) is defined as \( \mathbf{L}_1 = m \cdot 5 \mathbf{a}_G^{(1)} + n \cdot 5 \mathbf{a}_M^{(2)} = n \cdot 4 \mathbf{a}_M^{(1)} + m \cdot 4 \mathbf{a}_M^{(2)} \), where \( m, n \) are integers and related to the rotation angle \( \varphi \), and \( \mathbf{L}_2 \) is obtained by rotating \( \mathbf{L}_1 \) with 60° along counterclockwise direction [43–45]. The rotation angle \( \varphi \) is related to \((m, n)\) by

\[
\cos \varphi = \frac{1}{2} \frac{m^2 + n^2 + 4mn}{m^2 + n^2 + mn},
\]

and the unit cell of Moiré superlattice contains \( m^2 + n^2 + mn \) commensurate unit cells in each layer and \( N = 66(m^2 + n^2 + mn) \) C and M atoms. Figure 1(b) shows the atomic structures of (1, 2) twisted graphene and TMD with \( \varphi = 21.8^\circ \), where the blue parallelograms defined by \( \mathbf{L}_1 \) and \( \mathbf{L}_2 \) describes the Moiré superlattice.

3. Results and discussions

In this section, three methods are applied to enhance the proximity-induced SOC in the GNR, i.e. defects in the TMDNR, spatial interlayer edge coupling, and twist between the GNR and TMDNR, by breaking the bulk inversion symmetry of GNR/2D-TMD. Based on the largely enhanced SOC in the GNR, quasi-1D topological superconductor is realized on the GNR/TMDNR systems, and MZMs are manipulated at both ends of the GNRs.

3.1. Giant SOC induced by the bulk inversion asymmetry

Previous studies indicate that the bulk inversion asymmetry is contributed to the total SOC [25, 46, 47]. The bulk inversion asymmetry of the GNR/2D-TMD structure plays an important role for the magnitude of proximity-induced SOC in the GNR [25]. Thus, we firstly consider a GNR/TMDNR system where a narrow TMDNR. When the GNR’s Dirac point is close to the edge states of TMDNR, from 1.1 eV to 1.5 eV, where the GNR’s Dirac point is shifted upon from the band gap to the CBM of the TMDNR. The bulk inversion asymmetry of the GNR/2D-TMD structure plays an important role for the magnitude of the TMDNR. When the GNR’s Dirac point is close to the edge states of TMDNR, the spatial interlayer edge coupling, and twist between the GNR and TMDNR, by breaking the bulk inversion symmetry of GNR/2D-TMD. Based on the largely enhanced SOC in the GNR, quasi-1D topological superconductor is realized on the GNR/TMDNR systems, and MZMs are manipulated at both ends of the GNRs.

Recent works [6, 7, 11, 16, 17, 48] also show that the proximity-induced SOC in the graphene is sensitive to the relative band energies of 2D graphene and TMD which can be controlled by the gate voltage. Without loss of generality, we take a gate voltage to adjust the chemical potential of TMDNR (\( \mu_{TMD} \)). By fixing the chemical potential of the GNR (\( \mu_G = 0 \)), the relative energies between the CBM of GNR and the bands of TMDNR can be changed. Figure 2(c) shows the proximity-induced SOC in the GNR versus \( \mu_{TMD} \) from 1.1 eV to 1.5 eV, where the GNR’s Dirac point is shifted upon from the band gap to the CBM of the TMDNR. When the GNR’s Dirac point is close to the edge states of TMDNR, \( \lambda_G \) increases a little. With the further increase of \( \mu_{TMD} \), the GNR’s Dirac point moves away from the edge states of TMDNR, and the \( \lambda_G \) decreases. As the Dirac point is close to the CBM of the TMDNR, \( \lambda_G \) increases gradually and reaches...
Figure 2. (a) Schematic structure of unusual armchair GNR/TMDNR system with a narrow GNR lied in the middle of a broad TMDNR. (b) The bulk inversion symmetry case: the inequivalent \( K' \) and \( K \) valleys fold to the same points on the dashed line and so they will fold to the same points of the one-dimensional (1D) Brillouin zone (BZ) of the GNR/2D-TMD heterostructure. The hexagon shows the 2D TMD’s BZ, and the dashed line shows the direction in momentum space on which the 1D BZ of the GNR/2D-TMD heterostructure lies. If the inequivalent \( K' \) and \( K \) valleys fold to different points on the dashed line, the bulk inversion symmetry is broken [25]. (c) The band structure of the \((9 \times 15)\) GNR/TMDNR system shown in (a). The blue curves, black curves, red curves and green curves indicate the bands of GNR, bulk states, top edge states and bottom edge states of TMDNR, respectively. The chemical potential of GNR is set to zero, and the chemical potential of TMDNR is shifted to 1 eV to exhibit the Dirac core clearly. (d) The removal of degeneracy of Dirac core due to proximity-induced SOC. The spin up branch is shifted to the left, and the spin down branch is shifted to the right. \( E_{SO} \) is the energy splitting, and \( 2k_{SO} \) is the momentum splitting defining the magnitude of SOC. (e) Proximity-induced SOC in GNR varies with \( \mu_{TMD} \) of the GNR/TMDNR shown in (a). (Inset) Relative energy between the bands of the GNR and TMDNR at different \( \mu_{TMD} \). Maximum value \( \sim 6 \times 10^{-4} \), which is roughly two orders larger than the intrinsic SOC in the graphene. Significantly, \( \lambda_G \) is more sensitive to the TMD bulk states. We also calculated other narrow GNR and broad TMDNR systems, and similar variation of \( \lambda_G \) versus \( \mu_{TMD} \) are obtained with the same order of magnitude.

The obtained results are consistent with previous studies in graphene/TMD system [6, 16, 17, 48]. Similar results are obtained when we fix \( \mu_{TMD} \) and adjust the chemical potential \( (\mu_G) \) in the GNR.

The mechanism of this gate controlled proximity-induced SOC in the GNR can be understood by the low energy effective Hamiltonian \( H_{eff}(k) = H_G(k) + V_{eff}(k) \). \( H_G \) is the Hamiltonian of the GNR, and \( V_{eff} \) is the coupling between the GNR and TMDNR, which can be expressed as [15–17, 36]

\[
V_{eff}(k) = \sum_{\tilde{n},\tilde{k}} \frac{T_{\tilde{n}\tilde{k}}}{E_{\tilde{n}\tilde{k}} - E_{\tilde{n}\tilde{k}}},
\]

\[
T_{\tilde{n}\tilde{k}} = \langle \tilde{n}, k, s | H_T | \tilde{n}, \tilde{k} \rangle \langle \tilde{n}, \tilde{k} | H_T | k, X, s \rangle.
\]

\( T_{\tilde{n}\tilde{k}} \) describes the interlayer tunneling matrices, which is related to the \( p, d \) orbitals and spin \( s \). \( X \) is GNR’s \( p_z \) orbital; \( s \) is the spin index; \( E_G \) is the energy of GNR’s Dirac point; \( E_{\tilde{n}\tilde{k}} \) and \( | \tilde{n}, \tilde{k} \rangle \) are the eigenvalue and eigenstate of the interlayer coupling \( H_T \), respectively, with band index \( \tilde{n} \) and Bloch vector \( \tilde{k} \). When the Dirac point of GNR is close to the bulk states of TMDNR, \( E_G - E_{\tilde{n}\tilde{k}} \) approaches to zero, corresponding to a sharp SOC peak at relative energy. Therefore, we can observe the largest \( \lambda_G \) in the GNR when the valence band or the conduction band of the TMDNR is shifted toward the Dirac point of the GNR as shown in figure 2(e).

Although the SOC in the GNR has been enlarged roughly two orders to reach \( \sim 6 \times 10^{-4} \) by the gate voltage, it is still not enough to drive the GNR into the topological superconducting phase which is confirmed in the following section. In this view, we propose three ways to further increase the proximity-induced SOC in the GNR based on the gate controlled method, i.e. defects in the TMDNR, spatial interlayer edge coupling and twist between the GNR and TMDNR. The basic idea of these three methods is to break the bulk inversion symmetry of GNR/TMD, which has been proved an effective method to enlarge the SOC in the GNR [25].
3.1.1. Giant SOC induced by the defect of M-atom

We first consider the defect of M-atom in the TMDNR, where a point defect is introduced in every TMD supercell. The same middle coupled (9 × 15) GNR/TMDNR is still investigated except point defects are introduced in the TMDNR as shown in the top insets of figure 3(a). The bottom panel of figure 3(a) gives the band structure of the defective TMDNR, where lots of defective states appear comparing to figure 2(c). By tuning $\mu_{\text{TMD}}$ from 1.2 eV to 1.7 eV, the Dirac point of GNR is shifted from the midpoint of the band gap to the CBM of TMDNR, passing through several edge states. Due to the breaking of bulk inversion symmetry from the defect, the inequivalent $K$ and $K'$ valleys in the hexagonal BZ of 2D-TMD can no longer be folded to the same points of 1D BZ of the GNR/TMDNR system. As a result, the induced SOC is expected to be largely increased. Figure 3(b) presents the proximity-induced SOC in the GNR versus $\mu_{\text{TMD}}$ of the defective GNR/TMDNR system, where $\lambda_G$ increases monotonously. Two pieces of information are noticed. Firstly, $\lambda_G$ increases exponentially when $\mu_{\text{TMD}}$ tends to the CBM of TMDNR, and is not sensitive to the edge states of TMDNR. Secondly, the maximum $\lambda_G$ is significantly enhanced by roughly 30 times compared to that in the system without point defect as shown in figure 2(e). In addition, it is worth mentioning that the defect in GNR does not change the induced SOC because the bulk inversion symmetry of the GNR/2D-TMD is protected.

3.1.2. Giant SOC induced by the spatial interlayer edge coupling

The spatial interlayer edge coupling between the GNR and TMDNR is the second way to break the bulk inversion symmetry of GNR/2D-TMD, because here the wide TMDNR cannot be seen as a 2D structure. We still consider the (9 × 15) GNR/TMDNR system, but the narrow GNR is placed on one edge of the broad TMDNR as shown in the top panels of figure 3(c). The left panel of figure 3(c) shows the band structure of the 15-TMDNR, where the edges states contributed by the top and bottom edges are plotted by red and green curves, respectively. When $\mu_{\text{TMD}}$ is changed from 1.1 eV to 1.25 eV by a gate voltage, one top and one bottom TMD edge states are tuned to pass through the GNR’s Dirac point. $\lambda_G$ presents obvious dependence to the edge states other than the bulk states of TMDNR. If the GNR is coupled to the top edge of the TMDNR, the induced $\lambda_G$ raises sharply when GNR’s Dirac point is close the top edge state of TMDNR, see the red curve in the right panel of figure 3(c). Vice versa, when the GNR is coupled to the
bottom edge of the TMDNR, $\lambda_G$ increases obviously only when GNR’s Dirac point is close to the bottom edge state of TMDNR, see the green curve in the right panel of figure 3(c). The maximum $\lambda_G$ is roughly 20 times larger than that shown in figure 1(d) where the bulk inversion symmetry is protected. The large enhancement of $\lambda_G$ near edge states can also be understood from the low-energy effective Hamiltonian in equation (7). When the edge state of TMDNR gets close to GNR’s Dirac point, $E_G - E_{E_{z,T}}$ approaches to zero, corresponding to a sharp SOC peak at the relative energy. If the spin-splitting of the edge states in TMDNR is large, giant SOC in the GNR will be induced because the TMD edge states with larger spin-splitting would bring a greater modification of GNR’s band structure [6].

Obviously, the spatial interlayer edge coupling between the narrow GNR and broad TMDNR breaks the bulk inversion symmetry, and the edge states of TMDNR play a determinant role in obtaining giant proximity-induced SOC in the GNR. To verify this mechanism, we further consider a (15 × 15) GNR/TMDNR system, where both edges of the GNR are spatially coupled to both edges of the TMDNR as shown in the top panel of figure 3(d). As GNR’s Dirac point is shifted from the VBM to the CBM of TMDNR by tuning $\mu_{TMD}$, a series of peaks of $\lambda_G$ are observed when the graphene’s Dirac point passes through each edge band of the TMDNR, no matter top or bottom edge bands, as shown in the right panel of figure 3(d). In addition, the SOC due to the interaction between the Dirac point of the GNR and the bulk states of the TMDNR is much smaller than that contributed by the edge states of TMDNR. Another edge coupled (9 × 15) defective GNR/TMDNR is also investigated where the narrow GNR is placed on one edge of the wide defective TMDNR. Roughly the same giant enhancement of SOC in the GNR is also observed.

3.1.3. Giant SOC induced by the twist

The twist is the third method to enhance the proximity-induced SOC in the GNR. Without loss of generality, we take a narrow GNR and a broad TMDNR as an example, i.e. 6 Moiré superlattices as width of the twisted GNR and 10 Moiré superlattices as width of the twisted TMDNR, where the twist angle is 21.8° and periodic boundary condition is imposed along the $L_4$ direction (see figure 1(b)). The left panel of figure 3(e) presents the band structure of the twisted 10-TMDNR, which shows semiconducting property and exhibits rich edge states in the semiconducting gap. Compared to the untwisted TMDNR, more obvious spin-splitting of the edge states can be observed. For the middle coupled (6 × 10) twisted GNR/TMDNR, the bulk inversion symmetry of the GNR/TMD is broken, where the BZ of the 2D TMD is determined by the Moiré superlattice. By tuning $\mu_{TMD}$, the Dirac point of the GNR is shifted from the valence bands to the conduction bands of the twisted 10-TMDNR. As shown in the right panel of figure 3(e), $\lambda_G$ increases gradually when the Dirac point tends to the conduction band or valence band of TMDNR. The induced SOC in the twisted GNR is larger than that in the untwisted GNR shown in figure 2(e) by roughly 7 times. These novel behaviors are consistent with previous theoretical studies in 2D graphene/TMD system [15–17].

When the twisted six-GNR is placed to one edge of the twisted 10-TMDNR, the bulk inversion symmetry of GNR/TMD is further broken, and the edge states of TMDNR play a determinant role in increasing the induced SOC in the GNR. The behavior of the induced SOC in the twisted GNR are similar with the untwisted case in figure 3(c), but the magnitudes are enhanced heavily, as shown in the right panel of figure 3(f). If the twisted GNR is coupled to the top edge of the twisted TMDNR, the induced SOC raises sharply only when GNR’s Dirac point is close to the top edge states of the twisted TMD, and vice versa. The largest $\lambda_G$ can even reach 0.09, which is roughly 26 times larger than the maximum value shown in figure 3(e) of the middle coupled twisted system, and 150 times larger than the maximum value shown in figure 2(e) of the untwisted system with bulk inversion symmetry.

Finally, a brief summary is given. We confirm that the defects in TMDNR, spatial interlayer edge coupling, and twist between the GNR and TMDNR are three effective methods to enhance the proximity-induced SOC in the GNR by breaking the bulk inversion symmetry of the GNR/2D-TMD. Within these methods, the proximity-induced SOC in the GNR of the GNR/TMDNR systems can be enhanced by roughly 20 to 150 times. The induced large SOC can drive the GNR into a topologically superconducting phase in the presence of the Zeeman field and $s$-wave superconductivity.

3.2. Topological superconductivity and Majorana zero modes in GNR/TMDNR

As discussed above, giant proximity-induced SOC can be obtained by several methods through breaking the bulk inversion symmetry of GNR/2D-TMD. Moreover, if an in-plane magnetic field and $s$-wave superconductivity are further involved, the topological superconducting phases and MZMs can be realized in the GNR. Theoretically, the $s$-wave superconductivity in the GNR can be obtained by the proximity effect from superconducting TMD, such as NbSe$_2$ [52, 53]. The Hamiltonian of the topological superconductor can be expressed as

$$H = H_G + H_M + H_T + H_Z + H_{SC},$$

(8)
where $H_G$, $H_M$ and $H_T$ define the Hamiltonian of the GNR, TMDNR and their coupling, respectively, as shown in equations (1)–(3). $H_Z$ is the Zeeman term defining the in-plane magnetic field,

$$H_Z = V_Z \sum_{i,\alpha} \epsilon_{i,\alpha} \sigma_{\alpha}^\dagger \sigma_{\alpha} + \text{h.c.},$$

where $V_Z$ is the strength of the Zeeman interaction, and $\alpha = x, y$ is the direction of the in-plane magnetic field. $H_{SC}$ describes the $s$-wave superconductivity in the GNR as

$$H_{SC} = \Delta_G \sum_i c_i^\dagger c_i^\dagger + \text{h.c.}$$

Here $\Delta_G$ is the superconducting pairing potential in the GNR.

Firstly, we need to verify the existence of the topological superconducting phase in the GNR. Both the Berry phase $\phi$ based on periodic boundary condition [23, 24, 39] and Majorana polarization (MP) based on open boundary condition along the quasi-1D direction are calculated. The MP is defined as the magnitude of the integral of the MP vector over the spatial region $R$ as follows [54–58]

$$C = \frac{\sum_{j \in R} \langle \Psi | c_j^\dagger | \Psi \rangle}{\sum_{j \in R} \langle \Psi | \hat{r}_j | \Psi \rangle},$$

where $\hat{r}_j$ is the projection onto site $j$ and $c_j^\dagger \equiv C \hat{r}_j$. $\Psi$ is the real-space wave function in Nambu space defined as $\Psi = (\mu^\dagger, \nu^\dagger, -\nu^\dagger, \mu^\dagger)$, where $\mu$ and $\nu$ denote the electron and hole components, respectively. The local MP is simply the expectation value of the local particle–hole transformations:

$$\langle \Psi | c_j^\dagger | \Psi \rangle = -2 \sum_\sigma \epsilon_{\mu_\sigma} \epsilon_{\nu_\sigma}.$$

In general, we take $R$ to correspond to half of the system, divided usually along the longer length. When the system enters the topological superconducting phase, $C$ is confirmed equal to 1.

In figure 4(a), we shows the eigenvalues of a finite GNR (width $N_G = 2$ and length $N_x = 5000$) as the function of effective SOC. With the increase of the effective $\lambda_G$ in the GNR, the topological superconducting gap appears and increases. Meanwhile, MZMs only emerges above the critical SOC, which can also be verified by the MP. It demonstrates that enhancing the induced SOC is essential to realize MZMs in the GNR. From the above discussion, we know that the proximity-induced SOC in the GNR can be significantly enhanced by the defect in the TMDNR whether the middle coupling or the edge coupling. As the consequence, the quasi-1D topological superconducting GNR can be designed at arbitrary positions of the defective TMDNR, not just at the edges. As shown in figure 4(b), two MZMs appear at both ends of the GNR of the defective GNR/TMDNR system. Moreover, due to the overlap between the GNR’s Dirac point and the bulk state of the defective TMDNR as indicated in figures 3(a) and (b), the MZMs are also expanded into two ends of the TMDNR. Here, the existence of MZMs is verified by the Berry phase $\phi = \pi$ and MP $C = 1$. Similar results are found for the edge coupled or twisted GNR/TMDNR systems, which verify the importance of bulk inversion symmetry breaking in GNR/TMDNR systems.

Then, we investigate the topological superconducting property of the GNR in the edge coupled GNR/TMDNR system as shown in figure 4(c). The maximum value of proximity-induce SOC in the GNR is enlarged roughly 20 times comparing to that in the middle coupled GNR/TMDNR system with the same widths. Topological superconductivity is also proved. When the system enters the topological superconducting region, two MZMs appear at both ends of the GNR. Different from that shown in figure 4(b), the MZMs are localized inside the GNR but not appear at the ends of TMDNR. This is reasonable because only the edge states but not bulk states of the TMDNR are coupled with the Dirac point of the GNR accompanied with the induced maximum SOC. In the following, we consider a more complicated configuration, where two narrow GNRs are placed on the top and bottom edges of a very broad TMDNR, respectively, as shown in figure 4(d). We apply two gate voltages to control the chemical potential $\mu_1$ and $\mu_2$ of the top edge and the bottom edge of the TMDNR. By fine tuning the two gate voltages, the edge state from the top edge and the bottom edge can overlap and close to the Dirac point of the GNR as shown in figure 4(e). In this case, giant SOC can be induced in both GNRs. When including the Zeeman coupling and finite $s$-wave superconductor, quasi-1D topological superconductivity can be realized on each GNR. In figure 4(f), we present the numerical results of real space distribution of MZMs of the double edge coupled GNR/TMDNR system with $N_M = 96$ and $N_G = 2$. Each GNR is in the topological superconducting phase, and two pairs of MZMs, namely $\gamma_i/\gamma_i^\dagger$ and $\gamma_b/\gamma_b^\dagger$, appear at both ends of the top GNR and the bottom GNR, respectively.
Figure 4. (a) Eigenvalues versus effective SOC in a GNR with $N_G = 2$. (b) Defective $(1 \times 9)$ central coupled GNR/TMDNR system and its MZMs. (c) Pristine $(2 \times 12)$ edge coupled GNR/TMDNR system and its MZMs. (d) Two narrow GNRs are placed on both edges of a broad TMDNR. $\gamma_t$ and $\gamma_t^\dagger$ ($\gamma_b$ and $\gamma_b^\dagger$) are a pair of MZMs at top (bottom) edge of TMDNR, which can be tuned by changing the chemical potential $\mu_1$ and $\mu_2$ and in-plane magnetic field $B$. The arcs indicate the coupling of MZMs. (e) Band structure of the TMDNR in (d). The top and bottom edge states of the TMDNR are tuned to overlap and close to the Dirac point of GNR by applying spatially varied chemical potential $\mu_1$ and $\mu_2$. (f) Four Majorana corner states in (d). The parameters are: $V_Z = 3$ meV, $\Delta = 2$ meV.

Figure 5. (a) The topological phase diagram as function of $\mu_G$ and $V_Z$, $\Delta_G = 2$ meV. (b) The quantum device proposed, and multiple local gates are applied to transfer the MZMs.

Finally, we consider the transfer of the MZMs along the GNR. Figure 5(a) gives the topological phase diagram as a function of the chemical potential of the GNR and the Zeeman field. Numerical results show that the topological superconducting regions can be determined by $\mu_G$ and $V_Z$, and therefore the MZMs can be manipulated. The changing of $\mu_G$ and $V_Z$ can be realized by such an experimental device as shown in figure 5(b), where a series of local gates are set up along each GNR. By adjusting the gate voltages of any contacts, the GNR in this segment can enter or leave out the topological superconducting region, and the MZMs at the ends of the GNR are thus transferred. The transfer of MZM is a very useful method to ensure its spatial separation and localization. For example, if the TMDNR in figure 4(d) is not so broad compared to the two narrow GNR, such as $N_M = 12$ and $N_G = 2$, $\gamma_t(\gamma_t^\dagger)$ has strong hybridization with $\gamma_b(\gamma_b^\dagger)$ through the TMD substrate, forming zero-energy fermionic bound states, see the arcs in figure 4(d) [59]. By applying a local gate voltage on each GNR, the chemical potential of the ribbon ends are tuned into the topologically trivial phase, and the two hybridized MZMs are separated away from each other as shown in figure 5(b). This multi-GNRs/TMDNR system is a good platform to study the hybridization effect between MZMs. The hybridization will split the zero-bias peak, rule out Andreev bound states and quasi-Majorana states in experiments [60]. In addition, by coupling several narrow GNRs and one broad TMDNR, multiple MZMs can be realized and transferred in one TMD layer, which provides a useful platform for the MZM entanglement and quantum computation [61].
4. Experimental realization

Recent studies have reported the successful growth of TMDNRs with controlled width and length [62, 63]. NbS\textsubscript{2} and NbSe\textsubscript{2} possess superconductivity and strong SOC, which can be used as substrate to realize topological superconducting phases in the GNR [52, 53, 64]. Ferromagnetic insulator EuS [65] can provide magnetic field to the GNR by the proximity effect, and the Zeeman splitting in the bands of the GNR can be achieved with values comparable to those in Rashba nanowires. Therefore, the GNR sandwiched between NbSe\textsubscript{2} and EuS is a good candidate to realize the MZMs. Moreover, rich ways can be used to control and transfer the MZMs in the GNRs, such as the non-uniform chemical potential, strain and the interlayer distance [23, 24].

5. Conclusions

The bulk inversion asymmetry of the GNR/2D-TMD system is expected to result in giant proximity-induced SOC in the GNR. We introduce a TMDNR with finite width, and propose three methods to break the bulk inversion symmetry of GNR/2D-TMD structure, i.e. defects in the TMDNR, the spatial interlayer edge coupling, and the twist between the GNR and TMDNR. Numerical results show that point defect in the TMDNR can raise the SOC in the GNR by roughly 30 times compared to the pristine GNR/TMDNR system when the Dirac point of GNR is close to the bulk states of TMDNR. For the edge coupled GNR/TMDNR system, the edge states of TMDNR play a determinant role in the spin–orbit proximity effect, where the SOC in the GNR can be enhanced by roughly 20 times compared to the middle coupled GNR/TMDNR system with bulk inversion symmetry. In the twisted GNR/TMDNR system, the induced SOC can be enhanced by 150 times when the Dirac point of GNR is close to the edge states of TMDNR. The significantly enhanced SOC in the GNR is encouraging for the prospects of using GNR/TMDNR to realize quasi-1D topological superconductivity and MZMs. By the stacking several narrow GNR on one broad TMDNR, many pairs of MZMs can be generated in one system and transferred along GNRs by the gate voltages. This work confirms that the GNR/TMDNR systems with bulk inversion asymmetry are good platforms for the entanglement of MZMs and quantum computation.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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