Strain-controlled valley and spin separation in silicene heterojunctions

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I. INTRODUCTION

Silicene, a low-buckled monolayer-honeycomb lattice of silicon atoms, has been synthesized on metal surfaces1–3 and attracted extensive attention both theoretically4–6 and experimentally7,8 recently. Its low-buckled structure supports a relatively large spin-orbit coupling (SOC) and a sizable gap of 1.55 meV at the Dirac points K and K′9,10,11. The band gap of silicene can be modulated by applying a perpendicular electric field, thus inducing a topological phase transition as the electric field increases.11–13 The compatibility of silicene with silicon-based technology motivates many studies of interesting effects, such as the spin- and valley-Hall effects14–16, the quantum anomalous Hall effect17,18, valley-spin coupling19,20, and the strain-induced valley and spin separation in silicene systems21.

The existence of the spin-valley coupling makes silicene be a candidate for valleytronics. However, the SOC is weak compared with transition metal dichalcogenides (TMDs). The interplay of spin, valley and Berry phase related physics in TMDs, such as MoS2 and WSe2, can result in a valley-dependence spin Hall effect22,23. Compared with TMDs, it seems that silicene is not suitable for switching operations in valleytronics devices due to the weak SOC. Thus it is desirable to create a large band gap and SOC in silicene systems so as to catch up with TMDs in valleytronics. Recently, first-principles calculations show that the energy band can be significantly modulated by applying a strain in silicene systems24,25. The strain-induced band gap of silicene structures can reach the maximum value of 0.08 eV24. Obviously, the strain can induce a large band gap, which is comparable to that of TMDs and suitable for switching operations in valleytronics devices. Experimentally, one can realize a controllable strain in silicene via deposition onto stretchable substrates, similar to the strain effect in MoS226, or by exerting an external mechanical force.

However, the effect of the strain on the valley and spin separation in silicene systems has not been discussed previously. In this paper, we adopt the tight-binding mode-matching method and propose an efficient way to separate the Dirac fermions of different valleys, thus create a distinct spin separation by utilizing the strain and the electric field in silicene systems. Our results show that the valley- and spin-dependent electrons cannot be dispersed only by the electric field. Combining the strain and the electric field, one can realize an effective modulation of valley and spin-dependent transport by changing the amplitude or the stretch direction of the strain, without the need for ferromagnetic materials or magnetic fields. This phenomenon provides a novel route to effectively modulate the valley and spin polarizations of the silicene devices by utilizing the strain and the electric field.

Comparing with the tight-binding model, the Dirac theory is an effective approach which can only serve as a starting point for theoretical studies of transport in silicene. It has the advantage of yielding analytical results which capture the basic physical insights for certain problems, especially those with simplified system geometries. However, for a general consideration, e.g., for compli-
II. MODEL AND DISPERSION RELATIONS

We consider a low-buckled silicene sheet with zigzag direction along the axis $x$, in which the angle $\Omega$ describes the amplitude of the buckling with lattice constant being $a = 3.86\,\text{Å}$. In the central scattering region, the silicene sheet is stretched (or compressed) along the angle $\phi$ relative to the axis $x$, as shown in Fig. 1. Note that we assume there exists no strain outside the central scattering region. The silicene sheet can be described by the four-band second-nearest-neighbor tight-binding model [9, 10]

$$
H = \sum_{i\alpha} V_i c_{i\alpha}^\dagger c_{i\alpha} + \frac{t_{\sigma\sigma}(\xi)}{3\sqrt{3}} \sum_{(i,j)\alpha\beta} \nu_{ij} \sigma_{\alpha\beta} c_{j\beta}^\dagger c_{i\alpha}^\dagger
- \frac{2}{3} t_{\sigma\sigma}(\xi) \sum_{(i,j)\alpha\beta} \mu_i c_{i\alpha}^\dagger (\sigma \times \hat{d}_{ij})^z c_{j\beta}^\dagger
- \frac{t}{2} \sum_{(i,j)\alpha\beta} c_{i\alpha}^\dagger c_{j\beta} - \sum_{i\alpha} \mu_0 a_z E_z^i c_{i\alpha}^\dagger c_{i\alpha},
$$

where $c_{i\alpha}^\dagger (c_{i\alpha})$ refers to the creation (annihilation) operator with spin index $\alpha$ at site $i$, and $(i,j)/\{(i,j)\}$ run over all the nearest or next-nearest neighbor hopping sites. The first term is the on-site potential energy, the second term denotes the effective spin-orbit coupling with the hopping parameter $t_{\sigma\sigma}(\xi)$, where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the spin Pauli matrix operators, and $\nu_{ij} = \pm 1$ for the anticlockwise (clockwise) hopping between the next-nearest-neighboring sites with respect to the positive $z$ axis. The third term represents the Rashba spin-orbit coupling with $\mu_i = \pm 1$ for the A(B) site, where $d_{ij} = d_{ij}/|d_{ij}|$ refers to the unit vector connecting the two next-nearest-neighboring sites. The fourth term is the nearest-neighbor hopping with the transfer energy $t(\xi)$, where the vector $\xi$ is adopted to describe the elastic response for which deformations are affine [21]. The fifth term describes the contribution of the staggered sublattice potential, with $2a_z = 0.46\,\text{Å}$ being the distance of the two sublattice planes. The relaxed equilibrium values for the hopping parameters are $t^0(\xi) \approx 1.09\,\text{eV}$, $t_{\sigma0}^0(\xi) \approx 3.9\,\text{meV}$ and $t_{\sigma\sigma}^0(\xi) \approx 0.7\,\text{meV}$ [9, 10].

In the central scattering region, the silicene sheet is uniformly stretched (or compressed) along the angle $\phi$ relative to the axis $x$. Note that we assume there exists no strain outside the central scattering region. In the considered Cartesian coordinates, the tension $T$ can be written as $T = T(\cos \phi \hat{e}_x + \sin \phi \hat{e}_y)$. It is convenient to represent this tension in the principal coordinates $Ox'y'$, i.e., $T = T\hat{e}_{x'}$. In terms of the generalized Hooke’s law [23], the strain $\epsilon'_{ij}$ are related to the components of the compliance tensor, namely $\epsilon'_{ij} = T S_{ijxx}$, with the indices $i, j = x, y, z$. For the honeycomb lattice, we know that only five compliance tensor components are independent (i.e., $S_{xxx}, S_{xyy}, S_{xzz}, S_{zzz}, S_{xyy}$) [23]. Thus, the Poisson’s transverse ratio and perpendicular ratio are defined as

$$
\nu_\parallel = -S_{xyy}/S_{xxx}, \nu_\perp = -S_{zzz}/S_{xxx}. 
$$

FIG. 1: Schematic of the silicene heterojunction with an uniaxial strain, electric field and voltage potential in the central scattering region. The zigzag direction of the honeycomb lattice (x-y plane) is always parallel to the axis $x$, the tension is applied along the angle $\phi$ relative to the axis $x$, and the angle $\Omega$ is defined as between the Si-Si bond and the $z$ direction normal to the plane.
When the strain is applied to the low-buckled geometry, the lattice deformation will result in the change of the vectors $\xi_\ell$ ($\ell = 1, 2, 3$). Expanded in the first-order approximation, the strain-dependent vectors are given by $\tilde{\xi}_\ell = (1 + 1)\xi_\ell$, which thus modulates the hopping terms. Accordingly, we obtain the deformed bond length as follows

$$|	ilde{\xi}_1| = \left\{ \frac{\sqrt{2}}{10} \right\} a [2\cos^2 \phi + \sqrt{3} \sin 2\phi] (1 + \nu_\parallel)$$

$$+ (1 - 3\nu_\parallel - \frac{\nu_\perp}{6}) + \frac{5\sqrt{3}}{12} \} a,$$

$$|	ilde{\xi}_2| = \left\{ \frac{\sqrt{2}}{10} \right\} a [2\cos^2 \phi - \sqrt{3} \sin 2\phi] (1 + \nu_\parallel)$$

$$+ (1 - 3\nu_\parallel - \frac{\nu_\perp}{6}) + \frac{5\sqrt{3}}{12} \} a,$$

$$|	ilde{\xi}_3| = \left\{ \frac{2\sqrt{2}}{5} \right\} a [1 - \frac{\nu_\perp}{6} - \cos^2 \phi (1 + \nu_\parallel)] + \frac{5\sqrt{3}}{12} \} a.$$

The height is $h = \sqrt{2}(1 - \nu_\perp \epsilon_0)/12$. As the deformation is increased to $\epsilon_0 = 1/\nu_\perp$, the buckled structure is gradually stretched to a planar structure.

For the low-buckled silicene described by $s$ and $p$ orbitals, there are four types of hopping integrals $V_{ss\sigma}$, $V_{pp\sigma}$, $V_{pp\pi}$ and $V_{pp\pi}$. Within the Slater-Koster framework [29], the hopping processes between the neighboring sites depend only on the bond length and the relative angle $\Omega$. The hopping parameters in equation (11) can be calculated in terms of the formula given in Ref. [4], which considered the weak contribution of the angle $\Omega$ on the hopping processes. Under the two-center approximation adopted by Slater and Koster, the hopping integrals can be expressed as [30]

$$V_\mu(r_\ell) = \alpha_\mu r_\ell^{-\alpha_\mu} \exp(-\alpha_\mu r_\ell^{-\alpha_\mu}),$$

where $\mu$ refers to the four types of the hopping integrals, $r_\ell = |\tilde{\xi}_\ell|$ is the bond length, $\alpha_\mu (\mu = 1, 2, 3, 4)$ denotes the system parameters for silicene. So far, there are no microscopic evaluations of the four parameters for the silicene sheet from experiments and first-principle calculations. We slightly modify the parameters obtained from Environment-dependent tight-binding po-
When the electric field is in-plane, the energy bands are spin and valley-degenerate at the Dirac points K and K’ with the value of $(k_z, k_y, E)$. 

We first investigate the dispersion relation of the infinite-sized, homogeneous silicene sheet under the influence of the strain $\epsilon_0$ and the electric field $E_z$, as shown in Fig. 2. In the absence of the strain and the electric field, the energy band is spin and valley-degenerate and has a small band gap of about 8.2meV arising from the effective spin-orbit coupling. When the electric field is increased to the critical value $E_{zc} = t_{so}/a_z = 16.96$meVÅ [see Fig. 2(b)], we find that the band gap gradually approaches zero for up-spin electrons at K valley and down-spin electrons at K’ valley. Correspondingly, the spin and valley-degeneracy are broken by the electric field. Thus the electrons can become perfectly spin-up (spin-down) polarized at the K (K’) point under the influence of the electric field $E_{zc}$, which agrees well with the results obtained from the low-energy theory [11]. When the strain is applied to the silicene system, for example when $\epsilon_0 = 0.005$, the energy difference of the conduction band and the valence band increases to 5.6meV. With increasing amplitude of the strain to $\epsilon_0 = 0.05$, as shown in Fig. 2(d), the energy difference is significantly enlarged to about 100meV for the two valleys. Especially, the spin-polarization induced by the electric field is also suppressed, and the dispersion relation recovers the spin and valley degeneracy.

It is natural to consider whether the minima of energy profile for the two valleys still coincide at $k_y = 0$ in the presence of the strain. In order to clarify the effect of the strain on Dirac points, we plot the dispersion relations as a function of the wave vectors $k_x$ and $k_y$ for different strain strengths, as shown in Fig. 3. We can see that, when $\epsilon_0 = 0$, the Dirac points of K and K’ are located at the points with the wave vectors $(k_x, k_y) = (0.667, 0)$ and $(1.333, 0)$, respectively. Interestingly, the Dirac point K moves towards the positive direction of $k_y$ axis, while the Dirac point K’ moves towards the negative direction with the strain increasing from $\epsilon_0 = 0$ to 0.1. Thus, the application of strain results in a relative transverse shift of the two Dirac cones. At the same time, the Dirac points of K and K’ also move away from each other along the $k_x$ direction. Therefore, the dispersion relations in Fig. 2(c) and (d) are just representing a cut of...
the Dirac cone at \( k_y = 0 \), and that the energy difference between the conduction and valence bands depicted there are not the actual band gap. For comparison, we recall the graphene system where the strain can induce pseudo-magnetic fields greater than 300 Tesla \[31\]. This pseudo-magnetic field can be described by a gauge field \( A \) in the low-energy approximation \[32\]. Correspondingly, the Hamiltonian of the strained graphene sheet has the form \[33\] \[34\] \[35\] \[36\].

III. CALCULATION OF TRANSPORT PROPERTY

In order to calculate the transport property, we adopt the method formulated by Ando \[35\]. The silicene heterojunction is divided into cells indicated by an index \( \tau \), which represents a minimum repeating unit, as shown in Fig. 4. The source and drain are ideal leads that span the system. Since the leads have periodic structures, the matrices \( H_{\tau,\tau} \) and \( H_{\tau,\tau+1} \) are written as

\[
H_{\tau,\tau} = \begin{pmatrix} E_{\tau} - H_{\tau,\tau} & H_{\tau,\tau+1} \\ 0 & 0 \end{pmatrix}, \quad H_{\tau,\tau+1} = \begin{pmatrix} 0 & H_{\tau,\tau+1}^\dagger \\ 0 & 0 \end{pmatrix},
\]

for \( \tau = -\infty, \ldots, \infty \). If each cells contains \( N \) orbitals, \( \psi_\tau \) is a \( N \) dimensional vector including the wave-function coefficients of all orbitals for cell \( \tau \). \( H_{\tau,\tau} \) is the \( N \times N \) Hamiltonian matrix representing the hopping terms between sites within cell \( \tau \), \( H_{\tau,\tau\pm 1} \) is the \( N \times N \) Hamiltonian matrix connecting the sites between neighboring cells, which can be mapped from the tight-binding Hamiltonian in Eq. (1). Correspondingly, a pseudo-magnetic field can be described by a gauge field \( A \), which can be divided into propagating modes and evanescent modes in terms of the eigenvalues \[3\] \[4\].

After solving this equation, we obtain nontrivial solutions, which can be divided into propagating modes and evanescent modes in terms of the eigenvalues \[3\]. The eigenvalues of the propagating modes and the evanescent modes satisfy the conditions \( |\lambda(\pm)| = 1 \) and \( |\lambda(\pm)| \neq 1 \), respectively, with \(+/-\) referring to the right-going modes and left-going modes. When \( |\lambda(+)| < 1 \), the eigenvector is named as right-going evanescent modes, while the states with \( |\lambda(-)| > 1 \) associate with left-going evanescent modes. For the propagating states, in order to distinguish the right- and left-going modes, one needs to calculate their Bloch velocities

\[
v_n(\pm) = -\frac{2a}{h} \text{Im}[\lambda_n(\pm)\psi_n(\pm)^\dagger H_{\tau,\tau+1}^\dagger \psi_n(\pm)],
\]

where the sign of the velocities distinguishes right from left propagation. Accordingly, we can distinguish the valleys \( K \) and \( K' \) in terms of the wave vector \( k_x \) derived from the eigenvalue \( \lambda \). The first valley \( K \) is related to the longitudinal wave vector \( k_x \) in \( (0, \pi) \), whereas the second valley \( K' \) lies in the wave vector regime \( k_x \in (\pi, 2\pi) \) \[37\].

The general solution of the leads can be written as

\[
\psi_\tau = \psi_\tau^0 + \psi_\tau^1 = F_{\tau-\tau'}(+)\psi_\tau^0 (+) + F_{\tau-\tau'}(-)\psi_\tau^0 (-),
\]

where the matrices \( F(\pm) \) are defined as

\[
F(\pm) = \sum_n \lambda_n(\pm)\psi_n(\pm)^\dagger \psi_n(\pm),
\]

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\]

where the matrices \( F(\pm) \) are defined as

\[
F(\pm) = \sum_n \lambda_n(\pm)\psi_n(\pm)^\dagger \psi_n(\pm),
\]
where $\tilde{\psi}_n(\pm)$ are dual vectors, which satisfy the following relations

$$\tilde{\psi}_n(\pm)\psi_m(\pm) = \delta_{n,m}, \tilde{\psi}_n(\pm)\psi_m(\pm) = \delta_{n,m}. \quad (11)$$

Note that the eigenvectors are nonorthogonal.

Next we calculate the solutions of the scattering regions. By treating the effect of the leads as the bound-
ary conditions, the Schrödinger equation of the scattering region can be modified as

$$-iH_{\tau,\tau-1}\psi_{\tau-1} + (E - \epsilon_H')\psi_\tau - H_{\tau,\tau+1}\psi_{\tau+1} = \Delta_0\psi_\tau(+)\delta_{\tau,0}, \quad (12)$$

where the index of the cells becomes $\tau = 0, 1, \ldots, S, S + 1$. The renormalized Hamiltonian matrices are

$$H_{0,0} = H_{\tau,\tau} + H_{\tau,\tau+1}F_L^{-1}(-),$$
$$H_{S+S+1} = H_{\tau,\tau} + H_{\tau,\tau+1}F_R^{-1}(+),$$
$$H_{0+1, 0+1} = 0, H_{S+1,S+2} = 0, \quad (13)$$

and other Hamiltonian matrices are $H_{\tau,\tau'} = H_{\tau,\tau'}$ for the indexes $\tau, \tau' = 0, 1, \ldots, S, S + 1$. The source term is $\Lambda_0 = H_{\tau,\tau+1}[F_L^{-1}(+) - F_L^{-1}(-)]$ with $L/R$ referring to the left and right leads.

Eq. (12) gives a set of linear equations, which can be solved efficiently by using the block Gaussian elimination method. We can then obtain the transmission matrix elements $t_{n,m}$ by expanding the vector $\psi_{S+1}(\pm)$ in modes of the right lead

$$\psi_{S+1}(\pm) = \sum_{n}^{N} \psi_{R,n}(\pm)t_{n,m}, \quad (14)$$

where the incoming wave is chosen as one of the propagating modes of the left lead, namely $\psi_0(\pm) = \psi_{L,m}$. After running the vector $\psi_0(\pm)$ runs over all possible modes of the left lead, namely $\psi_{L,m}, m = 1, 2, \ldots, N$, the full transmission matrix can be obtained.

Accordingly, the total transmission can be written as

$$T_{LR}(k_y, E) = \sum_{n,m}^{N} \psi_{R,n}(+)|t_{n,m}|^2,$$
$$t_{n,m} = \tilde{\psi}_{R,n}(+)G_{S+1,0}^{-1}[G_{0,0}^{(0)}]^{-1}\psi_{L,m}(+), \quad (15)$$

where $G_{0,0}$ and $G_{S+1,0}$ refer to the Green’s function of the left lead and the full system, respectively, which can be obtained by using the iterative techniques of Green’s function approach.\cite{33}. After obtaining the Green’s functions, we can calculate the valley-resolved transmission in terms of the corresponding eigenvalues.

Utilizing the periodical boundary conditions at the transverse direction, we can introduce the wave vector $k_y$ into the Hamiltonian and effectively mimic the silicene sheet by using a silicene nanoribbon with zigzag chain number of $N_y = 2$ \cite{33}. The incident angle is defined as $\theta = \arcsin(k_y/k_F)$, where the Fermi wave vector $k_F$ can be obtained from the relation \cite{11}

$$E_F = \sqrt{\hbar^2v_F^2k_F^2 + \left(a_sE_z - \sqrt{l_{\hbar o} + a^2E_zh_2k_F^2}\right)^2}, \quad (16)$$

with $v_F = \sqrt{3}a\hbar/2$ being the Fermi velocity.

IV. RESULTS AND DISCUSSION

It is found that the valley-dependent and spin-dependent electrons cannot be dispersed by only the electric field. We thus consider the effect of the strain on the transport properties. In the central scattering region, the silicene sheet is uniformly stretched along the angle $\phi = 30^\circ$ relative to the axis $x$ with $E_z = 0$. When the strain is $\epsilon_0 = 0.005$, the transmission curve of K valley is deflected upwards, while the curve of K’ valley is deflected downwards, as shown in Fig. 5(a). Moreover, the maximum value of the transmission is significantly reduced to about 0.08 due to the effect of the strain.
It means that the strain can result in the separation of Dirac fermions of K and K’ valleys, which is similar with the deflection behavior induced by real magnetic fields in graphene systems [33–41].

In Fig. 6(b), we see that the spin-dependent transmission is decreased to about 0.052. However, the transmission profiles of up-spin and down-spin electrons are identical and symmetric with respect to normal incidence. Thus, the strain can separate the electrons of valleys K and K’ but cannot separate the up-spin and down-spin electrons.

In order to clarify the effect of the strain on the valley-dependent transport, we plot the transmission of valleys K and K’ as a function of the incident angle θ for different amplitudes of the strain, as shown in Fig. 6. We find that the transmission profile of K valley is deflected upwards with increasing strain from 0.004 to 0.01. When ε₀ = 0.01, the transmission of electrons is pushed towards the angular regime θ > 45° [see Fig. 6(a)]. Seen from the physical picture of view, the K-valley electrons will be scattered back the left region if the incident angle is smaller than a certain critical angle. Correspondingly, the transmission profile of the K’ valley is deflected downwards under the influence of the strain. The K’-valley electrons will be deflected back into the incident region when the incident angle is larger than a certain angle. When the strain is along the zigzag or armchair direction, namely φ = 0°, φ = 90° and φ = −90°, the transmission profiles have no deflection behavior, which is a distinct anisotropy behavior for the strain modulation of the valley current.

The above analysis show that strain can be utilized to separate the Dirac fermions of different valleys. Since silicene has a spin-valley correlation, it is thus natural to think that we can separate the electrons of different spins in the silicene sheet by applying the strain and an external electric field. Fig. 7 gives a clear picture of the strain modulation of spin and valley components. When E_z = 16.96meVÅ and ε₀ = 0.006, the transmission curves of valleys K and K’ still deflect upwards and downwards, respectively [see Fig. 7(a)]. The transmission profile of up-spin (down-spin) electrons is also obviously pushed upwards (downwards). This shows that the up-spin (down-spin) component is related to K (K’) valley. Therefore, one can separate the electrons of different spins into two opposite transverse directions, which can result in a strain-induced spin (valley) Hall effect in a suitable silicene device. This phenomenon is similar with the spin-valley Hall effect reported in monolayer graphene [42].

Similarly, the up-spin (down-spin) transmission curves are deflected upwards (downwards) when φ = 30° and φ = 45°, as shown in Fig. 8. However, when the angle is changed to negative values, namely φ = −30° and φ = −45°, the transmission profiles of up-spin and down-spin components are pushed downwards and upwards, respectively. When the strain is along the zigzag or armchair direction, the transmission profiles of two spin components are symmetrical with respect to the normal incident, so the up-spin and down-spin electrons cannot be separated at these strain configurations. These results imply that one can modulate the spin polarization by changing the stretching angle of the strain.

Since germanene also has a honeycomb geometry [13,14] and its Hamiltonian is the same as equation (1), germanene can be modeled by replacing the parameters with t = 1.3eV, t_σ = 43meV, t_H = 10.7meV and a_z = 0.33Å. The band gap induced by the spin-orbit couplings can reach 93meV [8], which can provide a significant modulation of spin- and valley-dependent properties. We think one can also observe the spin and valley separation in germanene systems due to its similar geometry and low-buckling structure. The numerical trends of the spin-valley separation due to strain in germanene systems is shown in Figs. 3–8 for silicene.

However, the parameters (e.g. the change in the bond length, and the α coefficients in the Slater-Koster integral) under the influence of strain and the electric field
would be different. Their exact values need to be determined e.g. by ab initio calculations, and currently they are not available in the literature, unlike for silicene. However, given the larger SOC values in germanene, we believe that one would require a relatively smaller amplitude of the strain to realize the same degree of valley and spin separation in comparison with silicene systems. This suggests that the strain-induced valley and spin separation can in general be observed in 2D materials with low-buckled honeycomb structures.

V. CONCLUSIONS

In summary, we have studied the effect of the strain and the external electric field on the dispersion relation and the transport property of a silicene heterojunction. It is found that the valley-dependent and spin-dependent electrons cannot be dispersed only by the electric field. In the presence of the strain, the transmission profiles can be deflected to two opposite transverse directions, thus resulting in the separation of valleys K and K’.

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Acknowledgments

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