Electron Delocalization in Gate-Tunable Gapless Silicene

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The application of a perpendicular electric field can drive silicene into a gapless state, characterized by two nearly fully spin-polarized Dirac cones owing to both relatively large spin-orbital interactions and inversion symmetry breaking. Here we argue that since inter-valley scattering from non-magnetic impurities is highly suppressed by time reversal symmetry, the physics should be effectively single-Dirac-cone like. Through numerical calculations, we demonstrate that there is no significant backscattering from a single impurity that is non-magnetic and unit-cell uniform, indicating a stable delocalized state. This conjecture is then further confirmed from a scaling of conductance for disordered systems using the same type of impurities.

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I. INTRODUCTION

It is well-known that a single-cone Dirac fermion is immune to backscattering and is thus hard to be localized. However, graphene has two Dirac cones (valleys), as required by the fermion doubling theorem. Consequently, in the presence of impurities, the inter-valley scattering from impurities cannot be strictly prohibited and this leads to remarkable backscattering, resulting in localization in two dimensions (2D). Upon this, it is essentially different from three-dimensional topological insulators (3DTIs), with just one Dirac cone for each surface.

Recently, silicene, which is the silicon version of graphene on a honeycomb lattice, has been an exciting subject. Due to its buckled structure, the spin-orbital coupling (SOC) is highly enhanced. With a perpendicular external electric field such structure also provides the tunability of the bulk gap. As the applied field increases, the gap closing and reopening indicates a topological phase transition between a 2DTI and a trivial band insulator. Exactly in the critical gapless state, where the low-energy electronic structure can be described by a massless Dirac Hamiltonian, forming two Dirac cones. The presence of various SOC interactions on the lattice results in rich spin textures around the Dirac points and eventually leads to profound behaviors in response to impurity scattering.

The most intriguing property of the gapless gated silicene, also the focus in this work, is the opposite spin polarization at different valleys, i.e., the valley-spin locking. Explicitly, the Dirac cone around K (K′) point is polarized with spin up (down), mainly originating from the intrinsic SOC between next nearest-neighbor (NNN) sites as well as broken inversion symmetry due to the external electric field. Thus, such phase is dubbed spin-valley-polarization metal (SVPM). Ideally assuming no Rashba SOC, the spin around each cone is fully polarized, and, contrary to graphene, inter-valley (also spin-flip) scattering from non-magnetic impurities is strictly prohibited by time reversal symmetry (TRS). Therefore, two Dirac cones in this system are effectively decoupled and consequently the two-component, single-flavor Dirac physics emerges. Now it is quite essential to ask if there can be any delocalized states in the strict sense under disorder. In addition, Rashba SOC, which includes spin-flip processes, is nevertheless inevitable in realistic silicene. Can it induce inter-valley scattering and lead to the breakdown of the single Dirac cone physics as well?

To answer these questions, in this paper, we systematically study the non-magnetic impurity scattering problem in the gapless system, designed to capture the physics of silicene and related materials, via numerical calculations. By comparing with various typical arrangements of SOCs, we found that 1) from the quasi-particle interference (QPI) pattern associated with single impurity, within a certain region of parameter space (low energy, small Rashba SOC, and moderate impurity scattering strength) for spin-valley-polarization metal, the “unit-cell impurity” will not give rise to significant inter- or intra-valley backscattering; 2) the positive beta function (defined below) in the disordered system further confirms the conclusion in 1) and suggests the existence of a truly delocalized state.

II. HAMILTONIAN AND EFFECTIVE THEORY

Silicene or the Ge, Sn, and Pb counterparts can be minimally described by a tight-binding model defined on a honeycomb lattice with energy scales $t \gg \lambda_{SO} >$
\[ H = t \sum_{\langle ij \rangle, \sigma} c_{i \sigma}^\dagger c_{j \sigma} + \frac{\lambda_{SO}}{3\sqrt{3}} \sum_{\langle \langle ij \rangle \rangle, \sigma \sigma'} \nu_{ij} c_{i \sigma}^\dagger s^z c_{\sigma' j \sigma'} - \frac{2 \lambda_R}{3} \sum_{\langle \langle ij \rangle \rangle, \sigma \sigma'} \mu_{ij} c_{i \sigma}^\dagger (s \times \hat{d}_{ij})^z c_{\sigma' j \sigma'} + \lambda_v \sum_{i, \sigma} \xi_i c_{i \sigma}^\dagger c_{i \sigma}. \]  

The first term describes the nearest-neighbor (NN) hopping, where \( c_{i \sigma}^\dagger \) creates an electron at site \( i \) with spin polarization \( \sigma \). The second term represents the intrinsic SOC between NNN sites, where \( s = (s_x, s_y, s_z) \) are the Pauli matrices for physical spins, and \( \nu_{ij} = (d_i \times d_j)_z/(d_i \times d_j) \) is \( \pm 1 \) for the two NN bonds connecting NNN sites \( i \) and \( j \). The third term is the NNN Rashba SOC, where \( \mu_{ij} = \pm 1 \) for the A and B sites, respectively, and \( \hat{d}_{ij} = d_{ij}/|d_{ij}| \) represent the unit vector of \( d_{ij} \) which connects NNN sites \( i \) and \( j \). The fourth term represents the staggered potential, and the strength \( \lambda_v = l_z E_z \) can be tuned by a perpendicular electric field \( E_z \) because of the buckling distance \( l_z \) between two sublattices. The model parameters for silicene are \( t = 1.04eV, \lambda_{SO} = 4.2meV, \lambda_R = 8.66meV \) and \( l_z = 0.035e\hat{A} \). Note that if we only keep the first term with \( t = 2.7eV \), Eq. 1 simply describes undoped graphene. Hereafter, we adopt \( t \) as the energy unit and lattice constant \( a \) (NNN distance) as the length unit.

Around two Dirac points at \( K(K') = (\pm \pi/3, 0) \) in \( k \)-space, the low-energy effective Hamiltonian for Eq. 1 with the basis \( (\psi_A^\dagger, \psi_B^\dagger, \psi_{A\dagger}, \psi_{B\dagger})^T \) reads

\[ H_{1}^{\eta}(q) = \begin{pmatrix} h_{1}^{\eta}(q) & g_{1}^{\eta}(q) \\ g_{1}^{\eta}(q) & h_{1}^{\eta}(q) \end{pmatrix}, \]  

\[ h_{1}^{\eta}(q) = \begin{pmatrix} -\eta \lambda_{SO} + \lambda_v \sqrt{\frac{2}{\xi^2}} (-\eta q_x - i q_y) \\ \sqrt{\frac{2}{\xi^2}} (\eta q_x + i q_y) \end{pmatrix}, \]  

\[ g_{1}^{\eta}(q) = \begin{pmatrix} \lambda_R (i q_x + q_y) & 0 \\ 0 & -\lambda_R (i q_x + q_y) \end{pmatrix}. \]  

where \( q \) is measured from the Dirac point, \( \eta = \pm 1 \) for \( K(K') \) point is the valley index, and \( h_{1}^{\eta}(q) \) is just the ideal Dirac fermion Hamiltonian for pseudo-spin, with Fermi velocity \( \sqrt{\frac{2}{\xi^2}} t \) and mass \( \lambda_v - \eta \lambda_{SO} \). Gating the system such that \( \lambda_v = \lambda_{SO} \) but with \( \lambda_R = 0 \), the full spin polarization of the valleys can be clearly seen: At valley \( K \), the spin-up bands are gapless forming a Dirac cone, in contrast to spin-down bands now separated by a gap \( \Delta_G = 2|\lambda_{SO} + \lambda_v|/\xi \) and thus out of the low-energy regime; at valley \( K' \) it is in opposite orientation due to TRS. The presence of considerable \( \lambda_R \) destroys this full spin polarization but the majority around each valley does not change. Such states with two massless Dirac cones will be the main focus throughout this work. Restricting \( \lambda_v = \lambda_{SO} \) (therefore \( \Delta_G = 0 \)) while allowing one to vary their strengths as well as the values of the Fermi level and \( \lambda_R \) in the system give rise to rich physics, which reflects the interplay among spin, sublattice (pseudo-spin), and valley degrees of freedom under non-magnetic impurity scattering.
III. QPI FROM SINGLE IMPURITY

The focus of the current study will be the effect of electronic scattering from impurity potentials. Impurity potentials can be induced by atomic substitution, surface adsorption or by the substrate under the 2D sample. Among various origins, the adsorption of different atoms for silicene has been discussed from ab initio calculations recently. In particular, it has been found that silicene tends to adsorb adatoms (including metal atoms) more strongly than graphene. Depending on which element is concerned, the adatom can sit on the “hill”, “valley”, “bridge” or “hollow” positions of the hexagonal ring respectively.

We first investigate the scattering from a single impurity, by calculating QPI pattern. The Green’s function for the clean system is $G^0(E, k) = G^0(E, k, k) \equiv \frac{1}{(E + i\gamma)I - H(k)}$, where $I$ is the identity matrix and $\gamma \ll 1$ is the energy broadening. Here we only consider a single impurity with potential $\sim \delta(x)$ in a definite unit cell so that the impurity matrix $V(k_1, k_2) = V$ is independent of $k$. The impurity induced Green’s function is expressed as

$$\delta G(E, k_1, k_2) = G^0(E, k_1)T(E, k_1, k_2)G^0(E, k_2).$$

The standard perturbation method gives

$$T(E) = [I - VT^0(E)]^{-1},$$

where $\Gamma^0(E) = \int \frac{d^2k}{(2\pi)^2} G^0(k, E)$. Now the Fourier transform of the induced local density of states is

$$\delta \rho(E, Q) = \frac{i}{2\pi} \int \frac{d^2k}{(2\pi)^2} \delta G(E, k, Q),$$

where $Q = k' - k$ and $\delta G(E, k, Q) = \text{Tr} (\delta G(E, k, k') - \delta G^*(E, k', k))$. The spectrum $\delta \rho(E, Q)$ in Eq. (7) is called the QPI pattern, which can also be obtained experimentally from the Fourier transformation of scanning tunneling microscopy (STM) measurements. This pattern provides an intuitive picture of scattering processes: Significant scattering processes will manifest peaks, consistent with the well-known fact that $V_a$ cannot induce backscattering for a massless ideal Dirac fermion. Notice that in the language of sublattice as pseudo-spin $\tau$, $V_a$ corresponds to a “unit-cell impurity” which is uniform within two sites of a unit cell. On the other hand, we also show the QPI for the “site impurity”, $V_b$, in Fig. (1e) as the black curve. Two peaks associated with intra-valley backscattering can be seen. This is not surprising because $V_b$ is a mass term for ideal Dirac fermion and destroys the pseudo-“TRS”, leading to a tendency towards localization. From results for an impurity with different weights of $V_a$ and $V_b$ also shown in Fig. (1e), it is interesting to notice that, a small weight ($r \approx 20\%$) of $V_a$ is sufficient to annihilate the significant backscattering peaks into the smooth background. In real space, an impurity with finite $V_a$ component corresponds to a long range one, with a smooth potential configuration within the unit cell. Such impurities can be dominant in graphene and therefore should also be easily realized experimentally for silicene. Moreover, the “hollow-type” and “bridge-type” adsorptions in silicene, which do not induce strong staggered potential, should also play such a role. In the rest of the paper, we will restrict ourselves to the discussions of unit-cell impurity $V_a$.

In the following, we will consider the full tight-binding $4 \times 4$ Hamiltonian $H(k)$, i.e., the $k$-representation of $H$.
in Eq. (1). For comparison purpose, we first take parameters $\lambda_{\text{SO}} = \lambda_v = \lambda_R = 0$ such that $H(\mathbf{k})$ describes graphene without SOC. Different from the case with ideal Dirac fermion Hamiltonian, $H(\mathbf{k})$ here has two important features: The existence of two spins and two valleys, and higher order corrections (trigonal warping) within each valley, as illustrated in Fig. 1(b). Given a unit-cell impurity potential,

$$V_a = V_0 s_0 \otimes \tau_0 = \text{diag}(V_0, V_0, V_0, V_0),$$

(9)

which is “non-magnetic” both for physical spin $s$ and pseudo-spin $\tau$, the corresponding QPI is shown in Fig. 1(f). It has very sharp peaks associated with inter-valley backscatterings between states with opposite $\mathbf{k}$ and velocity, as indicated by the green arrows. As in ordinary orthogonal disordered systems in 2D,\textsuperscript{20,21} this strong backscattering is responsible for the localization in graphene\textsuperscript{22} and weak 3D TIs.\textsuperscript{23} In short, the coupling between two Dirac cones (with opposite Berry curvatures)\textsuperscript{22} makes the physics rather trivial.

Armed with QPI studies from above two examples, we come to our main focus, gapless silicene with $\lambda_{\text{SO}} = \lambda_v = 0.5t$ for $H(\mathbf{k})$. Such large SOC is taken simply for giving enough space to extract out clear physics within our numerical precisions. No qualitative difference is expected as long as Fermi energy $E_F \in (-|\lambda_{\text{SO}} + \lambda_v|, |\lambda_{\text{SO}} + \lambda_v|)$, where the SPVM picture holds.

We first consider the spin conserved case $\lambda_R = 0$, where each valley is fully spin polarized [See Fig. 1(c)], therefore inter-valley scattering is prohibited. Indeed, with the same $V_a$ in Eq. (9), now the QPI in Fig. 1(g) is qualitatively different from that of graphene, but similar to that of the ideal Dirac fermion [Fig. 1(e)]. Moreover, there are no significant intra-valley backscattering peaks, either. The intra-valley features are almost isotropic in $Q$, as shown in the inset of Fig. 1(g), even though the full band structure is anisotropic around each Dirac point. It was argued that trigonal warping would lead to nonzero backscattering amplitude.\textsuperscript{22} However, our numerical results show that such backscattering is very weak and could be immersed in the continuum background of other scattering processes, reflected by the absence of associated distinguishable peaks. Therefore, the gapless silicene with broken inversion symmetry effectively exhibits the massless Dirac fermion physics, so long as the Fermi energy is not far from the Dirac point and the impurity strength is not strong (i.e., $|E_F| + |V_0| < E$, where $E \sim O(\lambda_{\text{SO}} + \lambda_v)$, the energy scale which protects the spin-valley-polarization metal phase). This is one of the important findings in this work. The absence of remarkable backscattering should signify a delocalized state to disorders, as will be numerically verified later.

Before entering into the discussion on disordered systems, two remarks are in order. First, in Figs. 1(c) and (g), with vanishing $\lambda_R$, inter-valley scattering is in fact suppressed \textit{a priori}. Nonzero $\lambda_R$, as to be the case in silicene, makes the spin-valley polarization imperfect [See Fig. 1(d)]. However, as shown in Fig. 1(h), it is remarkable to see that such Rashba term does not give rise to a significant inter-valley scattering, and thus the effective “single-valley Dirac physics” remains intact. This can be due to the following two intuitive reasons: 1) The NNN Rashba interaction makes no contribution at $K$ ($K'$) points and thus its effect is also expected to be small around $K$ ($K'$) points; 2) the full backward scattering, which relates inter-valley points, \textit{i.e.}, time-reversal partners (still with opposite spin polarizations under Rashba interaction), is difficult to happen through nonmagnetic impurity.

Second, further increasing a parameter such as $E_F$, impurity strength $V_0$, or $\lambda_R$ in the system is expected to enhance intra- and inter-valley scattering processes due to unavoidable contributions from higher order corrections and spin/valley mixing. Indeed, as clearly shown in Fig. 2, the QPI pattern changes at some point, indicating a transition from a delocalized to localized state beyond effective single-valley Dirac physics. For instance, in the case of very strong $\lambda_R$ in Fig. 2(i), although two states $|\mathbf{k}\rangle$ and $|\mathbf{-k}\rangle$ in different valleys (with exactly opposite spin orientations) cannot be coupled by a nonmagnetic impurity, the spin orientations in their neighborhoods will not be exactly opposite. Thus an inter-valley backscattering can be allowed due to the energy broadening $\gamma$.

IV. SCALING OF CONDUCTANCE: MULTIPLE IMPURITIES

So far, the scattering from a single impurity has been investigated. If the backscattering is effectively ignorable, does this really lead to delocalized state in disordered gapless silicene with unit-cell impurities? To confirm that it does, we perform a standard numerical scaling for disordered silicene. Disorder is added to the Hamiltonian $H$ as $\sum_{i, \sigma, i' \sigma'} c_i^{\sigma \dagger} c_{i'}^{\sigma'}$, where $\epsilon_i$ is a random number uniformly distributed within $(-W/2, W/2)$. Here $\epsilon_i$ is independent of spin due to TRS. If $\epsilon_i$ is further identical for two sites in each unit cell, then it corresponds to unit cell impurities $V_a$. In realistic silicene material, such impurities can be long range impurities as in graphene\textsuperscript{22} or the “hollow” and “bridge” types of adsorbed impurities as reported in Refs. 24 and 25. The intrinsic conductance $g$ is defined as $1/g = 1/g_L - 1/N_c$, where $g_L$ is the two-terminal quantum conductance, $N_c$ is the number of propagating channels and $1/N_c$ is the contact resistance.\textsuperscript{24} This $g$ is suitable for a numerical scaling\textsuperscript{19,24}

$$\beta = \frac{d\langle \ln g \rangle}{d\ln L},$$

(10)

where $\langle \cdots \rangle$ is the average over random ensemble, and $L$ is the spatial size of the sample with a fixed ratio of length and width. This scaling function $\beta$ is used as a criteria: $\beta < 0$ and $\beta > 0$ correspond to localized and delocalized states, respectively.
In Fig. 3 we plot \( \langle n \rangle \) as a function of size \( L \) (in logarithmic scale), where the slope represents \( \beta \). It can be seen from Figs. 3(a) and (b) that, for unit-cell impurities, apart from some fluctuations due to the smallness of conducting channels, \( \langle n \rangle \) is clearly increasing with increasing \( L \), suggesting a delocalized state with \( \beta > 0 \). These are consistent with our results of the absence of significant backscattering from the single impurity study, further confirming the robustness of the effective single-valley Dirac physics. Note that this is totally different from the case of graphene with the \( W = 2t \) [black curve in Fig. 3(c)], where the slope is negative. It has been found that for graphene, even long-range impurities cannot maintain a fully delocalized state with \( \beta > 0 \) because of inevitable inter-valley scattering. Of course, as in any lattice models, sufficiently strong disorder, for instance with \( V_0 > O(\lambda_{SO} + \lambda_v) \), will eventually localize all the electrons, as the red curve in Fig. 3(c) shows. Therefore, it is natural to expect rich localization-delocalization transition behavior in the parameter space spanned by \( E_R, W, \lambda_R \), and \( \lambda_{SO} (= \lambda_v) \). More details of such localization-delocalization transition, e.g., the universality, critical exponents, and global phase diagram will be discussed elsewhere.

Delocalized bulk states in the doped Kane-Mele model with nontrivial \( Z_2 \) topological nature were found in Ref. [23]. In that case, delocalized states can only appear when large (comparable to \( E_F \) and inversion-broken NN Rashba SOC is nonzero, making the system truly symplectic. Otherwise, the system is just decoupled into two gapped unitary subsystems, namely, two massive Dirac cones around \( K \) and \( K' \), where no states with \( \beta > 0 \) can be observed. This is indeed reasonable as a gapped Dirac cone has serious backscattering. In our case, however, the physics behind delocalization lies on either independent unitary subsystems, each of which owns a massless Dirac cone (zero NN Rashba SOC), or symplectic subsystems with two nearly independent gapless Dirac cones (nonzero NN Rashba SOC). The Dirac cones are already non-degenerate with almost fully spin polarization (along the \( z \) axis) as long as the inversion-symmetric, NNN \( \lambda_R \) interaction is small.

V. DISCUSSION AND CONCLUSION

The essence of this work is to reveal the physics behind the delocalization phenomenon, which can be understood from the picture of effectively decoupled gapless Dirac cones. This picture is valid in certain parameter ranges. Here we emphasize again the relevant energy scales important to any experimental demonstration for the delocalization in silicene, such as the presence of a robust Dirac point and linear dispersion in STM or the weak antilocalization in the magnetoresistance measurement. First, the gapless condition \( \lambda_v = l_z E_z = \lambda_{SO} \) gives the critical electric field \( E_z = \lambda_{SO}/l_z \sim 0.12\text{VÅ}^{-1} \), which is experimentally achievable. In this case, the half width of the energy window for spin-valley locking is \( |\lambda_{SO} + \lambda_v| = 2|\lambda_{SO}| \sim 8.4 \text{ meV} \). This range can be even larger in the Ge, Sn or Pb counterparts. On the other hand, such energy window is still small enough to keep the dispersion of Dirac fermions linear. Although NNN Rashba SOC breaks the perfect spin-valley locking, \( \lambda_R = 8.66 \text{ meV} \) is less than 1% of \( t \), and therefore this effect is very weak.

In summary, we reveal the essential transport properties via numerical simulations on a critically gated buckled honeycomb structure of silicene (and also suitable for the Ge, Sn, and Pb counterparts) under non-magnetic impurity scattering. In particular, as long as \( |E_F| + |V_0| < E \) with \( E \), an energy scale of the order of \( \lambda_{SO} + \lambda_v \), we find: 1) QPI by a single unit-cell impurity shows no significant backscattering, suggesting an effective single-valley Dirac physics, in spite of weak trigonal warping. 2) The robustness of such delocalized state is further confirmed by the positiveness of the \( \beta \) function for a disordered system, even in the presence of Rashba
SOC. Our finding sheds a new light on constructing high mobility silicene-based electronic devices. Moreover, we believe our result is also insightful to relevant systems such as a 2D MoS$_2$ and a cold-atom system with arranged SOC.

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