

Disorder driven transition beyond two-component, single-flavor Dirac physics in silicene

Partha Goswami

Deshbandhu College, University of Delhi, Kalkaji, New Delhi-110019, India

The corresponding author's e-mail address: physicsgoswami@gmail.com

Abstract. We consider the topological insulator (TI) phase of silicene in the presence of an applied electric field E_z perpendicular to its plane. These are assembly of Dirac fermions on a low-buckled 2D hexagonal lattice. The buckled structure generates a staggered sub-lattice potential between silicon atoms at A sites and B sites for the applied field. The starting point of our investigation is the Hamiltonian involving the Dirac kinetic energy, a mass gap term, and the spin-orbit coupling. Tuning of E_z allows for rich behaviour starting from a TI state to a band insulator(BI)with a valley-spin-polarized metal (VSPM) at a critical value in between. As long as the impurity potential strength V_0 is of the same order as the intrinsic spin-orbit coupling (SOC) $t_{so}(\sim 4 \text{ meV})$, VSPM phase is protected. The effective “two-component, single-flavor Dirac physics” remains valid in this phase. The increase in V_0 , however, leads to the disappearance of this phase due to enhanced scattering processes, i.e. the out-of-plane electric field driven topological insulator to metal transition, being predicted for our system, will not be observable when the impurity potential is very high. The enhancement in SOC (t_{so}) or the Rashba spin-orbit coupling effect (t_2), however, does not lead to such a scenario. **PACS numbers:** 71.90.+q, 73.43.-f, 73.22.-f, 71.70.Ej, 85.75.-d.

1.Introduction The purpose of this communication is to report the investigation of the effect of elastic scattering by non-magnetic impurities on the transition of Dirac fermions on a low-buckled 2D hexagonal lattice, such as the stand-alone, low-buckled monolayer silicene(MLS), from a topological insulator to a semi-metal. Fleurence et al.[1] possibly have succeeded for the first time in preparing silicene on Si wafers via a conductive ceramic zirconium diboride (ZrB_2) buffer layer, though there have been quite a few independent silicene synthesis reports around the same time on the conducting substrate, such as that of the epitaxial silicene sheets on silver (111) [2,3]. It must be mentioned here that the existence of Dirac fermions itself in silicene is somewhat speculative due to the lack of direct evidences from experiment [4,5]. The MLS is basically a semimetal because the valence and conduction bands touch at the Fermi level. It consists of a honeycomb lattice of silicon atoms with two sub-lattices made of A and B sites. The states near the Fermi energy are π orbitals residing near the Dirac points K and K' at opposite corners of the hexagonal Brillouin zone. The silicene sheet, in fact, has linear band crossing at the K and K' symmetry points. As in graphene, thus, the charge carriers in silicene behave like relativistic particles with a conical energy spectrum and Fermi velocity $v_F \approx 10^6 \text{ m-s}^{-1}$. The honeycomb lattice of the system is distorted due to a larger (than carbon) ionic radius of silicon atom and forms a buckled structure as already mentioned. The A and B sites per unit cell form two sub-lattices separated by a perpendicular distance, say, 2ℓ . The structure generates a staggered sub-lattice potential $2\ell E_z$ between silicon atoms at A sites and B sites for an applied electric field E_z . Silicene has a larger spin-orbit coupling (SOC) induced gap than graphene due to its buckled structure. Remarkably, the silicene exhibits a tunable band gap due to the applied electric field E_z perpendicular to the system-plane. Tuning of E_z , allows for rich behavior varying from a topological insulator(TI) to a band insulator(BI) with a valley spin-polarized metal (VSPM) at



a critical value (E_c) in between. In fact, at the critical point with $(E_z/E_c) = 1.00$, the gap of one of the spin-split band pairs of a K point closes to give a Dirac point while the other pair is gapped. At the other K point the same spin band is gapped; other spin band, of course, is gapless. This is an out-of-plane electric field induced TI to semi-metal transition. This is also referred to as the topological phase transition (TPT). In this paper we show that, as long as the non-magnetic impurity scattering strength is moderate, i.e. the potential strength is of the same order or less than t_{so} , the VSPM phase characterized by the spin-valley locking is protected. The TPT is, however, remarkably sensitive to the impurity strength in the moderate and high doping regimes. The increase in the impurity strength leads to the effective disappearance of the VSPM phase. In fact, the strong impurity strength robs away the topological protection of the VSPM, and related two-component Dirac physics, against dissipation and fluctuations, and forces the system's entry into an unexplored domain. In this communication we do not explore *terra incognita*, we rather engage ourselves in the preliminary task of the integration of the impurity effect, via Green's function and Dyson's equation, into the single-particle spectrum which is the starting point of the investigation of the thermodynamic properties, the transport properties, and so on. The paper is organized as follows: In Sec. 2, a brief outline of the tight binding model of silicene is given and the low-energy excitation spectrum is obtained. This is followed by the presentation of the Born scattering approximation in Sec.3. The t-matrix approximation to deal with the impurity problem is also discussed in Sec.3. The renormalized single-particle excitation spectrum for the finite chemical potential is obtained. The result concerning sensitivity of TPT to the impurity potential could be found at the end of this section.

2. The Low-energy Excitation Spectrum We start with the silicene single-particle low energy Hamiltonian [6,7,8] expressed in terms of 4×4 Dirac matrices (γ^μ) in the Weyl basis as

$$H_{Si} = \sum_{\delta k, \alpha, \beta} c_{\delta k, \alpha}^\dagger \mathcal{H}_{\alpha\beta}(\delta k) c_{\delta k, \beta} \quad (1)$$

where

$$\begin{aligned} \mathcal{H}(\delta k) = & \left(\frac{\hbar v_F}{a} \right) \times [a v^x \delta k_x + a v^y \delta k_y] + \xi \left(\frac{\hbar v_F}{a} \right) \times [(\boldsymbol{\ell} \mathbf{E}'_z) \times (\gamma^5 \gamma^z \gamma^0) + \mathbf{t}'_{so} \times (\gamma^5 \gamma^z \gamma^0 \gamma^5)] \\ & - (M / \left(\frac{\hbar v_F}{a} \right)) \gamma^5, \quad \Delta_z = E'_z = \frac{E_z}{\left(\frac{\hbar v_F}{a} \right)}, \quad \Delta_{soc} = \mathbf{t}'_{so} = \mathbf{t}_{so} / \left(\frac{\hbar v_F}{a} \right), \end{aligned} \quad (2)$$

$$c_{\delta k, \beta} = (a_{\delta k \uparrow}, b_{\delta k \uparrow}, a_{\delta k \downarrow}, b_{\delta k \downarrow}), \quad v^x = \xi (\gamma^5 \gamma^0 \gamma^x + i \mathbf{t}'_2 \gamma^z), \quad v^y = (\gamma^5 \gamma^0 \gamma^y - \xi t'_2 \gamma^5 \gamma^z). \quad (3)$$

The operators $a_{\delta k, \sigma}$ and $b_{\delta k, \sigma}$ ($\sigma = \uparrow, \downarrow$), respectively, with momentum δk and spin σ correspond to the annihilation operators for the electronic density in the two independent sub-lattices A and B. The first term is the Dirac kinetic energy and the second is a symmetry-breaking term. It breaks the sub-lattice symmetry of the silicene's honey-comb structure and generates a gap. The stronger spin-orbit coupling (SOC) $\mathbf{t}_{so}$ in H_{Si} has its origin in the buckled structure of the system. The term t_2 corresponds to a Rashba spin-orbit coupling effect in H . Here ξ is the iso-spin index with $\xi = +1$ and $\xi = -1$ for the Dirac points $\mathbf{K}$ and $\mathbf{K}'$. The exchange field ' M ' arises due to proximity coupling to a ferro-magnet such as depositing Fe atoms to the silicene surface or depositing silicene to a ferromagnetic insulating substrate. The 2×2 version [9] of H_{Si} , valid when the valley mixing is absent, is given by

$$\mathcal{H}_{reduced}(\xi, s_z, \delta k) / \left(\frac{\hbar v_F}{a} \right) = [\xi a \sigma^x \delta k_x + a \sigma^y \delta k_y + (\xi s_z \Delta_{SOC} + \Delta_z) \sigma^z - (\mu a / v_F \hbar) \sigma^0]. \quad (4)$$

for the exchange field $M = 0$. Here, the Pauli matrices σ^x , σ^y , σ^z and σ^0 act in the space of the electrons' amplitudes on orbitals attributed to the independent A and B sub-lattices. In this approximation, the pseudo-spin is in the foreground; the iso-spin (described by the index $\xi = \pm 1$) and the real spin (described by an index $s_z = \pm 1$) are in the back-ground. It is, thus, possible to describe electrons by the

effective two-component wave function. In the remaining part of the paper we shall confine ourselves to this two-component description. Here $\mu' = (\mu a / v_F \hbar)$ is the dimensionless chemical potential of the fermion number. In writing this Hamiltonian we have ignored the low-buckled (silicene) structure generated intrinsic Rashba terms, as $t'_2 \ll \Delta_{SOC}$.

We find that the dimensionless spin-split bands close to a Dirac point are given by $E_k^{(U,L)} = \pm [(a|\delta k|^2 + \{\xi s_z \Delta_{SOC} + \Delta_z\}^2)^{1/2} - \mu']$. Thus, the effect of the intrinsic SOC together with the electric field is to impart fermions with mass as they correspond to an effective staggered sub-lattice potential $V(\xi, s_z) = \{\Delta_{SOC} + \xi s_z \Delta_z\}$. The presence of a perpendicular electric field gives rise to spin-split gapped bands about K points at $(E_z/E_c) < 1$. The plot of silicene dispersion as a function of $(k_x a)$ for $(k_y a) = 0$ and $(E_z/E_c) = 1$ for the valley index $\xi = +1$ is shown in Figure 1. At $(E_z/E_c) = 1$, if, the dispersion for

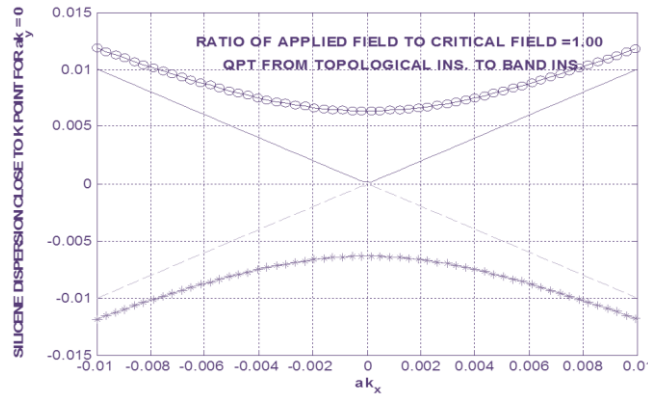


Figure 1: The presence of spin orbit coupling and a perpendicular electric field gives rise to spin-split bands about the Dirac points, with two gaps one of which may be tuned to zero at $(E_z/E_c) = 1.00$ as shown above.

the valley (or iso-spin) index $\xi = +1$ and the spin $\downarrow$ is gapless, it is gapped for $\xi = +1$ and the spin $\uparrow$. Similarly, for $\xi = -1$ and the spin $\uparrow$ if the dispersion is gapless, for $\xi = -1$ and the spin $\downarrow$, it is gapped. The gapless situation corresponds to a valley-spin-polarized metal (VSPM) as, for $\xi = +1$ the possible spin state is $\downarrow$ only, and for $\xi = -1$ the possible spin state $\uparrow$ only. For $(E_z/E_c) > 1$, the spectrum becomes fully gapped again but the system is again an insulator albeit without a gapless spectrum of edge states for the electrons protected by topology [10,11]. The transition requires the presence of the Kane-Mele [11] spin-orbit (SO) coupling t'_{so} and the electric field.

3. t-Matrix Approximation The effect of elastic scattering by non-magnetic impurities and spin-orbit scattering involve the calculation of the total self-energy $\Sigma(\mathbf{k}, \omega_n)$ in terms of the Matsubara frequencies ω_n , which alters the single-particle excitation spectrum in a fundamental way. In the Green's function (GF) matrix $\check{G}(\mathbf{k}, \omega_n)$ we insert [9] the self-energy corresponding to the scattering by the former with the help of the Dyson's equation $(\check{G}(\mathbf{k}, \omega_n))^{-1} = (\check{G}_0(\mathbf{k}, \omega_n))^{-1} - \Sigma(\mathbf{k}, \omega_n) \sigma^0$, where the unit matrix σ^0 acts on the sub-lattice space. The non-interacting GF matrix may be formally given by $(\check{G}_0(\mathbf{k}, \omega_n))^{-1} \sim (i\omega_n \sigma^0 - \bar{H}_{reduced}(\xi, \mathbf{s}_z, \delta k))$. We first consider only the contribution of the Fig.2(a). Assuming the elastic scattering by impurities weak, impurities are alike, and the distribution is random, we may write it as

$$\Sigma^{(I)}(\mathbf{k}, \omega_n) \sigma^0 = n_0 \sum_{\mathbf{k}'} |V_0(\mathbf{k} - \mathbf{k}')|^2 G_{\alpha, \alpha}(\mathbf{k}', \omega_n) \sigma^0 = \Sigma_0^{(I)}(\mathbf{k}) \sigma^0 \quad (5)$$

where $V(|\mathbf{q}|)$ is the Fourier coefficient of the impurity potential $V(\mathbf{r})$. The function $\Sigma_0^{(I)}(\mathbf{k})$ is the first order contribution independent of ω_n , for $\Sigma_0^{(I)}(\mathbf{k}) = -n_0 \rho_0 (i\omega_n) \sum_{\mathbf{k}'} |V_0(\mathbf{k} - \mathbf{k}')|^2 (\pi / |\omega_n|) = [-i\omega_n / (2|\omega_n| \tau_k)]$, where the reciprocal quasi-particle lifetime (QPLT) $\tau_k^{-1} = 2\pi n_0 \rho_0 \sum_{\mathbf{k}'} |V_0(\mathbf{k} - \mathbf{k}')|^2$. The full propagator may now be written as

$$G^{(Full)}_{\alpha, \alpha}(\mathbf{k}, \omega_n) \approx u_k^2 [i\omega_n - \epsilon_r(\mathbf{k}) + i(1/4\tau_k) + \mu]^{-1} + v_k^2 [i\omega_n + \epsilon_r(\mathbf{k}) + i(1/4\tau_k) + \mu]^{-1}, \quad (6)$$

where the renormalized excitation spectrum is given by $\epsilon_r(k) = [\{(a|k|)^2 + \{\Delta_{SOC} + \xi s_z \Delta_z\}^2\} - (\eta/16 \tau_k^2)]$, $\eta = \{(a|k|)^2 / (V^2 + (a|k|)^2)\}$. The chemical potential μ , according to the Luttinger rule, is given by the equation $1 = [d(\mathbf{k}a) \sum_v \rho^{(v)}_{Fermi}(\mathbf{k}) \times (\exp(\beta(\epsilon_r^{(v)}(\mathbf{k}) - \mu)) + 1)^{-1}]$ where $\rho^{(v)}_{Fermi}(\mathbf{k})$ is the Fermi energy density of states, and $[d(\mathbf{k}a) \rightarrow -\pi \int_{-\pi}^{+\pi} (d(k_x a)/2\pi - \pi \int_{-\pi}^{+\pi} (d(k_y a)/2\pi$, and $\beta = (k_B T)^{-1}$.

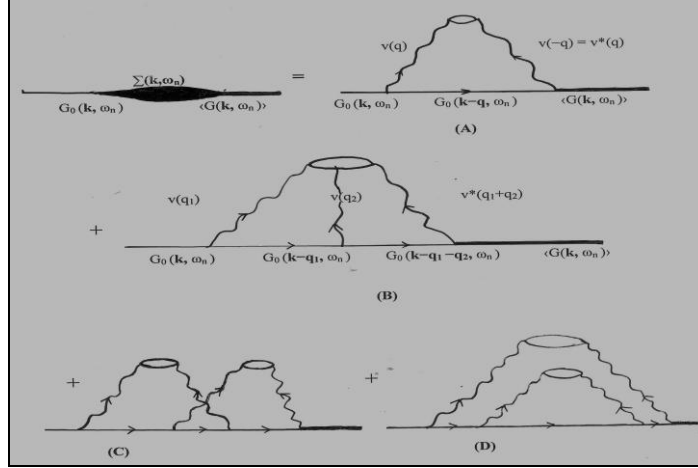


Figure 2. A few diagrams contributing to the self-energy. The wiggly lines carry momentum but no energy. The total momentum entering each impurity vertex, depicted by a slim ellipse, is zero.

Next, we consider the quasi-particle scattering problem within the t-matrix approach[12,13]. As a necessary step, assuming low concentration of impurities, one may include the contributions of all such diagrams in Fig.2 which involve only one impurity vertex. This gives the equation to determine the total self-energy $\Sigma(\mathbf{k}, \omega_n)$ involving vertex function $\Gamma_0(\mathbf{k}, -\mathbf{q}, \omega_n)$ which in turn is given by the Lippmann-Schwinger equation:

$$\Sigma_e(\mathbf{k}, \omega_n) = n_0 \sum_{\mathbf{k}'} V_0(\mathbf{q}) G_{\alpha, \alpha}(\mathbf{k} - \mathbf{q}, \omega_n) \Gamma_0(\mathbf{k}, -\mathbf{q}, \omega_n) \quad (7)$$

where the vertex function

$$\Gamma_0(\mathbf{k}, -\mathbf{q}, \omega_n) = V_0(-\mathbf{q}) + \sum_{\mathbf{q}'} V_0(\mathbf{q}' - \mathbf{q}) G_{\alpha, \alpha}(\mathbf{k} - \mathbf{q}', \omega_n) \Gamma_0(\mathbf{k}, \mathbf{q}', \omega_n). \quad (8)$$

This is the t-matrix approximation. Upon using the optical theorem for the t-matrix [13] one may write $\Sigma(\mathbf{k}, \omega_n) = i \text{Im} \Gamma(\mathbf{k}, \mathbf{k}, \omega_n) = -i \omega_n / (2|\omega_n| \dot{\Gamma}_k)$ where $\dot{\Gamma}_k^{-1} = 2\pi \rho_0 \sum_{\mathbf{k}'} (n_0 |\Gamma_0(\mathbf{k}, \mathbf{k}')|^2)$. Thus the effect of the inclusion of contribution of all the above mentioned diagrams is to replace the Born approximation for scattering by the exact scattering cross-section for a single impurity, i.e. $\tau_k^{-1} \rightarrow \dot{\Gamma}_k^{-1}$. Since $G_{\alpha, \alpha}(\mathbf{k}, \omega_n)$ and $V_0(\mathbf{k})$ are known, one can determine $\dot{\Gamma}_k^{-1}$ in terms of $V_0(\mathbf{k})$.

3.1 Result The increase in the non-magnetic impurity scattering strength leads to the disappearance of the VSPM phase: Upon considering the case ($s_z = -1, \xi = +1$), for example, one finds the gap closing at the $\mathbf{K}$ point, i.e. $E_{renorm}(\mathbf{k}, s_z = -1, \xi = +1) \approx \pm (a|k|)$ for $\mu' = 0$, the critical Δ_z given by $\Delta_{zc} \approx [(t'_{so})^2 + (at'_2 |\delta k|)^2]^{1/2} - (\pm 1/4 \dot{\Gamma}_k) \{(a|k|)^2 / (V^2 + (a|k|)^2)\} \approx -(\pm 1/4 \dot{\Gamma}_k)$, and the gapped spectrum at the $\mathbf{K}'$ point, i.e. $E_{renorm}(\mathbf{k}, s_z = -1, \xi = -1) \approx \pm [(a|k|)^2 + 4\Delta_z^2]^{1/2}$. The fact that $\{(\frac{\hbar v_F}{a}) a|k| / ((\frac{\hbar v_F}{a} V)^2 + (\frac{\hbar v_F}{a}) a|k|)^2\} \approx 1$ and $t'_{so})^2 + (a t'_2 |\delta k|)^2 \ll (1/16 \dot{\Gamma}_k^2)$ implies that $\Delta_{zc} \approx \mp 1/4 \dot{\Gamma}_k$. The result means the ‘so-called’ gap closing could be accessed only at an unreasonably high value of the applied electric field. The inescapable conclusion is TPT does not remain protected in the presence of strong non-magnetic impurities. With $t_2 \ll t_{so}$ we do not also expect the Rashba coupling to play a major role in the VSPM issue.

References

- [1] A. Fleurence, R. Friedlein, T. Ozaki, H. Kawai, Y. Wang, Y. Yamada-Takamura, Phys. Rev. Lett. 108, 245501 (2012).
- [2] P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M. C. Asensio, A. Resta, B. Ealet, and G. Le Lay, Phys. Rev. Lett. 108, 155501 (2012).
- [3] L. Chen, C. Liu, B. Feng, X. He, P. Cheng, Z. Ding, S. Meng, Y. Yao, and K. Wu, Phys. Rev. Lett. 109, 056804 (2012).
- [4] C.-L. Lin, R. Arafune, K. Kawahara, M. Kanno, N. Tsukahara, E. Minamitani, Y. Kim, M. Kawai, and N. Takagi, Phys. Rev. Lett. 110, 076801 (2013).
- [5] S. Cahangirov, M. Audiffred, P. Tang, A. Iacomino, W. Duan, G. Merino, and A. Rubio, Phys. Rev. B 88, 035432 (2013).
- [6] M. Ezawa, New J. Phys. 14, 033003 (2012).
- [7] M. Ezawa, Phys. Rev. Lett. 109, 055502 (2012).
- [8] M. Ezawa, Phys. Rev. Lett. 110, 026603 (2013).
- [9] V.P. Gusynin, S.G. Sharapov, and A.A. Varlamov, Phys. Rev. B 90, 155107 (2014).
- [10] N.D. Drummond, V. Zolyomi, and V.I. Fal'ko, Phys. Rev. B 85, 075423 (2012).
- [11] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 2268-01 (2005).
- [12] C. Bena, S. Chakravarty, J. Hu, and C. Nayak, Phys. Rev. B 69, 134517 (2004).
- [13] G. Rickayzen, Green's Functions and Condensed Matter (Academic Press Inc. Ltd., London, 1980), chap. 4, p. 105.