Supplementary information for "Valley polarized Quantum Hall effect and topological insulator phase transitions in silicene" by M. Tahir and U. Schwingenschlögl

I. MODEL

We model silicene by an effective Hamiltonian in the xy-plane. An external magnetic field (0, 0, B) is applied perpendicular to the silicene sheet, taking into account SOI effects and electric field. Dirac fermions in buckled silicene obey the two-dimensional graphene-like Hamiltonian

$$H_s^\eta = v(\sigma_x \mathbf{p}_x - \eta\sigma_y \mathbf{p}_y) - \eta s\Delta_{SO}\sigma_z + \Delta_z\sigma_z. \tag{1}$$

Here, $\eta = +/-$ denotes K/K', $\Delta_z = lE_z$, where E_z is the uniform electric field applied perpendicular to the silicene sheet with $l = 0.23$ Å. In addition, (σ_x, σ_y, σ_z) is the vector of Pauli matrice, and v denotes the Fermi velocity of the Dirac fermions. Spin up ($\uparrow$) and down ($\downarrow$) is represented by $s = +1$ and -1, respectively. Moreover, $\mathbf{p} = \mathbf{p} + e\mathbf{A}/c$ is the two dimensional canonical momentum with vector potential $\mathbf{A}$, and c is the speed of light. Using the Landau gauge with vector potential (0, Bx, 0) and diagonalizing the Hamiltonian given in Eq. (1) we obtain the eigenvalues

$$E_{s,n,t}^\eta = t\sqrt{n\hbar^2\omega^2 + (\Delta_{SO} - \eta s\Delta_z)^2}. \tag{2}$$

Here, $t = +/-$ denotes the electron/hole band, $\omega = v\sqrt{2eB/\hbar}$, and n is an integer. The corresponding eigenfunctions for the K point with spin up and $n > 0$ are

$$\Psi_{\uparrow,n,+}^K = \frac{\exp[ik_y y]}{\sqrt{L_y}}\begin{pmatrix} \sin\theta_{+,+}/2\phi_n \\ -i\cos\theta_{+,+}/2\phi_{n-1}\end{pmatrix}, \Psi_{\uparrow,n,-}^K = \frac{\exp[ik_y y]}{\sqrt{L_y}}\begin{pmatrix} \cos\theta_{+,+}/2\phi_n \\ i\sin\theta_{+,+}/2\phi_{n-1}\end{pmatrix} \tag{3}$$

with $\theta_{\eta,s} = \tan^{-1}\frac{\omega\sqrt{n}}{(\Delta_{SO}-\eta s\Delta_z)}$. The usual harmonic oscillator eigenstates are denoted as ϕ_n where n is the index of the Landau level. The corresponding solutions for the K point with spin down and $n > 0$ are

$$\Psi_{\downarrow,n,+}^K = \frac{\exp[ik_y y]}{\sqrt{L_y}}\begin{pmatrix} \cos\theta_{+,-}/2\phi_n \\ -i\sin\theta_{+,-}/2\phi_{n-1}\end{pmatrix}, \Psi_{\downarrow,n,-}^K = \frac{\exp[ik_y y]}{\sqrt{L_y}}\begin{pmatrix} \sin\theta_{+,-}/2\phi_n \\ i\cos\theta_{+,-}/2\phi_{n-1}\end{pmatrix}. \tag{4}$$

The corresponding eigenvalues and eigenfunctions for the $n = 0$ state are obtained as

$$E_{s,0}^\eta = -(s\Delta_{SO} - \eta\Delta_z) \tag{5}$$

and

$$\Psi_{s,0}^{K} = \frac{\exp[ik_y y]}{\sqrt{L_y}} \begin{pmatrix} \phi_0 \\ 0 \end{pmatrix}, \Psi_{s,0}^{K'} = \frac{\exp[ik_y y]}{\sqrt{L_y}} \begin{pmatrix} 0 \\ \phi_0 \end{pmatrix}. \quad (6)$$

The eigenfunctions for the K' point can be obtained by exchanging electron and hole eigenstates in the K point solution with ϕ_{n-1} interchanged by ϕ_n.

II. HALL CONDUCTIVITY

The Hall conductivity σ_{xy} is obtained from the nondiagonal elements of the conductivity tensor, given by

$$\sigma_{xy} = \frac{i\hbar e^2}{L_x L_y} \sum_{\xi \neq \xi'} f(E_\xi)[1 - f(E_{\xi'})] \langle \xi | v_x | \xi' \rangle \langle \xi' | v_y | \xi \rangle \frac{(1 - e^{\beta(E_\xi - E_{\xi'})})}{(E_\xi - E_{\xi'})^2}. \quad (7)$$

where $f(E_\xi) = (\exp(\frac{E_\xi - E_F}{k_B T}) + 1)^{-1}$ is the Fermi Dirac distribution function. Since $f(E_\xi)[1 - f(E_{\xi'})](e^{\beta(E_\xi - E_{\xi'})}) = f(E_{\xi'})[1 - f(E_\xi)]$, we obtain

$$\sigma_{xy} = \frac{i\hbar e^2}{L_x L_y} \sum_{\xi \neq \xi'} [f(E_\xi) - f(E_{\xi'})] \frac{\langle \xi | v_x | \xi' \rangle \langle \xi' | v_y | \xi \rangle}{(E_\xi - E_{\xi'})^2}. \quad (8)$$

Since the x and y components of the velocity operator are $v_x = \frac{\partial H}{\partial p_x}$ and $v_y = \frac{\partial H}{\partial p_y}$, where $H_s^\eta = v(\sigma_x p_x - \eta \sigma_y p_y) - \eta s \Delta_{SO} \sigma_z + \Delta_z \sigma_z$, we have $v_x = v\sigma_x$ and $v_y = -\eta v \sigma_y$. Hence

$$\langle \xi' | v_x | \xi \rangle = \frac{-itv \sin \theta_{\eta,s}}{2} (\delta_{n-1,n'} - \delta_{n,n'-1}) \quad (9)$$

and

$$\langle \xi | v_y | \xi' \rangle = \frac{tv \sin \theta_{\eta,s}}{2} (\delta_{n-1,n'} + \delta_{n'-1,n}). \quad (10)$$

The matrix elements of the velocity operator are nonzero only when $\eta = \eta'$ and $n' = n \pm 1$. Since $|\xi\rangle \equiv |\eta, s, n, t, k_y\rangle$, there is a summation over k_y which, with periodic boundary conditions for k_y, gives

$$\sum_{k_y} \to \frac{L_y}{2\pi} \int_{-L_x/2l^2}^{L_x/2l^2} dk_y = \frac{L_x L_y}{2\pi l^2}, \quad (11)$$

for only one occupied state. If both states are occupied we have to multiply with a factor of 2 and $s = s'$. Substituting the values of the velocity matrix elements in Eq. (8) yields

$$\sigma_{xy} = \frac{\hbar e^2 v^2}{\pi l^2} \frac{t^2 \sin^2 \theta_{\eta,s}}{4} \sum_{\xi \neq \xi'} \frac{[f(E_\xi) - f(E_{\xi'})]\,[\delta_{n-1,n'} - \delta_{n,n'-1}]}{(E_\xi - E_{\xi'})^2}. \quad (12)$$

Since $E_\xi \equiv E^\eta_{s,n,t} = t\sqrt{n\hbar^2\omega^2 + (\Delta_{SO} - \eta s\Delta_z)^2}$ we obtain

$$(E_\xi - E_{\xi'})^2 = \left[t\sqrt{n\hbar^2\omega^2 + (\Delta_{SO} - \eta s\Delta_z)^2} - t'\sqrt{n'\hbar^2\omega^2 + (\Delta_{SO} - \eta s\Delta_z)^2}\right]^2. \tag{13}$$

Plugging Eq. (13) into (12), we obtain

$$\sigma_{xy} = \frac{\hbar e^2 v^2}{\pi l^2} \sum_{s,t,t',n,n',\eta} \frac{\sin^2\theta_{\eta,s}}{4\hbar^2\omega^2} \frac{[f(E^\eta_{s,n,t}) - f(E^\eta_{s,n',t'})]\,[\delta_{n-1,n'} - \delta_{n,n'-1}]}{\left[t\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} - t'\sqrt{n' + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right]^2} \tag{14}$$

To solve Eq. (14) for $t, t' = +,+$ and $+,-$ the summation in the above equation for $n' = n+1$ is written as

$$\sum_{s,\eta} \frac{[f(E^\eta_{s,n,+}) - f(E^\eta_{s,n+1,+})]}{\left(\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} - \sqrt{n + 1 + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2} + \frac{[f(E^\eta_{s,n,+}) - f(E^\eta_{s,n+1,-})]}{\left(\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} + \sqrt{n + 1 + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2}. \tag{15}$$

Note that the $n' = n - 1$ contribution vanishes as this corresponds to a transition to filled states. Equation (15) can be further simplified to yield

$$\sum_{s,\eta} \left\{ \begin{array}{l} \left(\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} + \sqrt{n + 1 + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2 [f(E^\eta_{s,n,+}) - f(E^\eta_{s,n+1,+})] \\ + \left(\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} - \sqrt{n + 1 + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2 [f(E^\eta_{s,n,+}) - f(E^\eta_{s,n+1,-})] \end{array} \right\}$$
$$\Big/ \left\{ \begin{array}{l} \left(\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} - \sqrt{n + 1 + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2 \\ \times \left(\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} + \sqrt{n + 1 + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2 \end{array} \right\}. \tag{16}$$

For $t, t' = -,+$ and $-,-$ we have

$$\sum_{s,\eta} \frac{[f(E^\eta_{s,n,-}) - f(E^\eta_{s,n+1,+})]}{\left(-\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} - \sqrt{n + 1 + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2} + \frac{[f(E^\eta_{s,n,-}) - f(E^\eta_{s,n+1,-})]}{\left(-\sqrt{n + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2} + \sqrt{n + 1 + (\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2}. \tag{17}$$

Equation (17) can be further simplified to yield

$$\sum_{s,\eta}\left\{\begin{array}{c}\left(-\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}+\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2[f(E^\eta_{s,n,-})-f(E^\eta_{s,n+1,+})]\\ +\left(-\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}-\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2[f(E^\eta_{s,n,-})-f(E^\eta_{s,n+1,-})]\end{array}\right\}$$
$$/\left\{\begin{array}{c}\left(-\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}-\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2\\ \times\left(-\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}+\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2\end{array}\right\}. \tag{18}$$

For the numerator of Eq. (16) we obtain

$$\begin{aligned}&\left(\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}+\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2[f(E^\eta_{s,n,+})-f(E^\eta_{s,n+1,+})]\\ &+\left(\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}-\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2[f(E^\eta_{s,n,+})-f(E^\eta_{s,n+1,-})]\\ &=\left[\begin{array}{c}2n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2\\ +2\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\end{array}\right][f(E^\eta_{s,n,+})-f(E^\eta_{s,n+1,+})]\\ &+\left[\begin{array}{c}2n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2\\ -2\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\end{array}\right][f(E^\eta_{s,n,+})-f(E^\eta_{s,n+1,-})]\end{aligned} \tag{19}$$

and for the numerator of Eq. (18)

$$\begin{aligned}&\left(-\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}+\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2[f(E^\eta_{s,n,-})-f(E^\eta_{s,n+1,+})]\\ &+\left(-\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}-\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2[f(E^\eta_{s,n,-})-f(E^\eta_{s,n+1,-})]\\ &=\left[\begin{array}{c}2n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2\\ -2\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\end{array}\right][f(E^\eta_{s,n,-})-f(E^\eta_{s,n+1,+})]\\ &+\left[\begin{array}{c}2n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2\\ +2\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\end{array}\right][f(E^\eta_{s,n,-})-f(E^\eta_{s,n+1,-})].\end{aligned} \tag{20}$$

The denominators of Eqs. (16) and (18) are the same and simplify to

$$\begin{aligned}&\left(\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}+\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2\\ &\times\left(\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}-\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\right)^2\\ &=\left((\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2-(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2-1\right)^2.\end{aligned} \tag{21}$$

Grouping terms such as $+,+$ and $+,-$ for t and t' that contain $f(E^{\eta}_{s,n,+})$ leads to the cancellation of the factor $2\sqrt{n+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}\sqrt{n+1+(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2}$ in Eq. (19). The same holds for the $-,-$ and $-,+$ terms in Eq. (20). Now using Eqs. (17), (18), (19), (20), and (21) in Eq. (14) we obtain

$$\sigma_{xy}=\frac{\hbar e^2v^2}{\pi l^2}\sum_{s,n,\eta}\frac{\sin^2\theta_{\eta,s}}{4\hbar^2\omega^2}\times\begin{bmatrix}[4n+2(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2+2+2(\frac{\Delta_{SO}-\eta s\Delta_z}{\hbar\omega})^2]\\ \times[f(E^{\eta}_{s,n,+})-f(E^{\eta}_{s,n+1,+})+f(E^{\eta}_{s,n,-})-f(E^{\eta}_{s,n+1,-})]\end{bmatrix}. \quad (22)$$

The spin and valley dependent Hall conductivity given in Eq. (22) is further simplified to

$$\sigma_{xy}=\frac{e^2}{2h}\sum_{s,n,\eta}\sin^2\theta_{\eta,s}[2n+2(\frac{\Delta_{SO}-s\eta\Delta_z}{\hbar\omega})^2+1] \quad (23)$$
$$\times[f(E^{\eta}_{s,n,+})-f(E^{\eta}_{s,n+1,+})+f(E^{\eta}_{s,n,-})-f(E^{\eta}_{s,n+1,-})]$$

where $f(E^{\eta}_{s,n,t})=(\exp(\frac{t\sqrt{n\hbar^2\omega^2+(\Delta_{SO}-\eta s\Delta_z)^2}-E_F}{k_BT})+1)^{-1}$ is the Fermi Dirac distribution function. Equation (23) is the same as for graphene for $\Delta_{SO}=\Delta_z=0$. In the limit of zero temperature, Eq. (23) can be further simplified to

$$\sigma_{xy}=\frac{2e^2\sin^2\theta_{\eta,s}}{h}\left(2n+1+2(\frac{\Delta_{SO}-s\eta\Delta_z}{\hbar\omega})^2\right). \quad (24)$$

III. LONGITUDINAL CONDUCTIVITY

To obtain the longitudinal conductivity, we assume that the electrons are elastically scattered by randomly distributed charged impurities, as it has been shown that charged impurities play a key role in the transport properties of silicene near the Dirac point. This type of scattering is dominant at low temperature. If there is no spin degeneracy, the longitudinal conductivity is given by

$$\sigma^{\text{long}}_{xx}=\frac{e^2}{L_xL_yk_BT}\sum_{\xi,\xi'}f(E_\xi)[1-f(E_{\xi'})]W_{\xi\xi'}(E_\xi,E_{\xi'})(x_\xi-x_{\xi'})^2. \quad (25)$$

Here, $f(E_\xi)$ is the Fermi Dirac distribution function, with $f(E_\xi)=f(E_{\xi'})$ for elastic scattering, k_B is the Boltzmann constant, and E_F is the chemical potential. $W_{\xi\xi'}(E_\xi,E_{\xi'})$ is the transmission rate between the one-electron states $|\xi\rangle$ and $|\xi'\rangle$, and e is the charge of the electron. Conduction occurs by transitions through spatially separated states from x_ξ to $x_{\xi'}$, where $x_\xi=\langle\xi|\,x\,|\xi\rangle$. The londitudinal conductivity arises as a result of migration of the cyclotron orbit due to scattering by charged impurities. The scattering rate in Eq. (25) is written as

$$W_{\xi\xi'}(E_\xi, E_{\xi'}) = \frac{2\pi N}{L_x L_y \hbar} \sum_q |U_q|^2 |F_{\xi\xi'}(r)|^2 \delta(E_\xi - E_{\xi'}) \delta_{k_y, k'_y + q_y} \tag{26}$$

with $q = \sqrt{q_x^2 + q_y^2}$, $u = l^2(q_x^2 + q_y^2)/2 = l^2 q^2/2$, and the impurity density N. The Fourier transform of the screened impurity potential is $U_q = U_0/\sqrt{q^2 + k_0^2}$, where $U_0 = e^2/4\pi\epsilon_0\epsilon_r$. Moreover, k_0 is the screening wavevector, ϵ_r the static dielectric constant of the material, and ϵ_0 the dielectric permittivity. $F_{\xi\xi'}(r) = \langle\xi| \exp(iqr) |\xi'\rangle$ are the form factors and $|\xi\rangle \equiv |n, s, t, \eta, k_y\rangle$. Neglecting the mixing of the Landau level index, i.e., taking $n = n'$, and noting that $\sigma_{xx}^{\text{long}} = \sigma_{yy}^{\text{long}}$ for screened impurity scattering ($k_0 >> q$) we can ignore the q dependence. We have $(x_\xi - x_{\xi'})^2 = l^4 q_y^2$ and $q_y = q_\perp \sin\zeta$. Since the wavefunction oscillates around lk_y, we have $\sum_{k_y} \to \frac{L_y}{2\pi} \int_{-L_x/2l^2}^{L_x/2l^2} dk_y = \frac{L_x L_y}{2\pi l^2}$ and, using cylindrical coordinates, $\sum_q \to \frac{L_x L_y}{4\pi^2 l^2} \int_0^{2\pi} d\zeta \int_0^\infty du$. The form factor $|F_{\xi\xi'}(r)|^2$ can be evaluated from the matrix element to yield $|F_{nn}(u)|^2 = \exp(-u)\left(\sin^2\theta_{\eta,s} L_n(u) + \cos^2\theta_{\eta,s} L_{n-1}(u)\right)^2$ for $n = n'$. Inserting these factors in Eq. (26) the longitudinal conductivity after evaluating the integral can be written as

$$\sigma_{xx}^{\text{long}} = \frac{e^2}{h} \frac{N}{2l^2\hbar\omega k_B T} \frac{U_0^2}{k_0^2} \sum_{n,s,t,\eta} \left[\begin{array}{c} (2n + 1\eta)\sin^4\theta_{\eta,s} + (2n - 1\eta)\cos^4\theta_{\eta,s} \\ +2n \sin^2\theta_{\eta,s} \cos^2\theta_{\eta,s} \end{array} \right] f(E_{s,n,t}^\eta)[1 - f(E_{s,n,t}^\eta)], \tag{27}$$

where $f(E_{s,n,t}^\eta) = (\exp(\frac{t\sqrt{n\hbar^2\omega^2 + (\Delta_{SO} - \eta s\Delta_z)^2} - E_F}{k_B T}) + 1)^{-1}$. Equation (27) is the same as for graphene in the limit $\Delta_{SO} = \Delta_z = 0$.