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Spin- and valley-dependent commensurability oscillations and electric-field-induced quantum Hall plateaux in periodically modulated silicene

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We study the commensurability oscillations in silicene subject to a perpendicular electric field \( E_z \), a weak magnetic field \( B \), and a weak periodic potential \( V = V_0 \cos(Cy) \). The field \( E_z \) and/or the modulation lift the spin degeneracy of the Landau levels and lead to spin and valley resolved Weiss oscillations. The spin resolution is maximal when the field \( E_z \) is replaced by a periodic one \( E_z = E_0 \cos(Dy) \). The study is an extension of that for graphene but contrary to it, in which the SOI is very weak. We explore the influence of SOI on the commensurability or Weiss oscillations10 in silicene in which the SOI is very weak. Silicene has a intrinsic SOI that leads to a gap of 1.55 meV.3 This gap can be further controlled by an external electric field facilitated by the buckled structure of silicene. This and its compatibility with silicon-based technology led already to additional quantum Hall conductivity plateaux arise due to spin and valley intra-Landau-level transitions. © 2014 AIP Publishing LLC.

A monolayer honeycomb structure of silicon, called silicene, has been predicted to be stable1 and several attempts have been made to synthesize it.2 Silicene has Dirac cones similar to those of graphene but contrary to it, in which the spin-orbit interaction (SOI) is very weak, silicene has a strong SOI due to its low-buckled geometry and large atomic intrinsic SOI that leads to a gap of 1.55 meV.2 This gap can be further controlled by an external electric field \( E_z \) and is facilitated by the buckled structure of silicene. This and its compatibility with silicon-based technology led already to many studies, reviewed in Ref. 4, such as the spin-Hall effect3,5 and the capacitance of an electrically tunable silicon device.6 Moreover, very recent theoretical studies predict the stability of silicene on nonmetallic surfaces such as graphene,7 boron nitride or SiC,8 and in graphene-silicene-graphene structures.8

Since the SOI can lead to spin-resolved transport, pertinent to quantum computing, it is worth studying it further in silicene and contrast the results with those for graphene in which the SOI is very weak. We explore the influence of SOI on the commensurability or Weiss oscillations10 in silicene in the presence of the field \( E_z \), of a perpendicular magnetic field \( B \), and of a weak periodic potential \( V(y) = V_0 \cos(Cy) \). These oscillations result from the fact that modulation-broadened Landau levels (LLs) have a bandwidth that oscillates with weak \( B \) and expresses the commensurability between the modulation period and the cyclotron diameter at the Fermi level. The study is an extension of that for a two-dimensional electron gas (2DEG)11 and of that for graphene.12,13 In addition, we consider a periodic field \( E_z = E_0 \cos(Dy) \). If one or two such modulations is present, the spin degeneracy is lifted and leads to spin-dependent commensurability oscillations when \( B \) is varied; the lifting is stronger for a periodic field \( E_z \).

Unmodulated silicene. The one-electron Hamiltonian, near the \( K \) and \( K' \) valleys, in a magnetic field \( B \), in the Landau gauge for the vector potential \( A \), is

\[
H = v_F (\pi_x \sigma_x - \tau \pi_y \sigma_y) - (\tau \sigma_z \lambda_{\text{so}} - \ell E_z) \sigma_z, \tag{1}
\]

after shifting the wave vectors \( k_x \) and \( k_y \) by \( eA_y/\hbar, \mu = x, y \), i.e., by setting \( \mathbf{P} = \mathbf{p} + eA \), with \( \mathbf{p} \) is the momentum operator and \( e \) is the electron charge. Here, \( v_F \) is the Fermi velocity, \( \tau = +(-) \) is the \( K (K') \) valley index, \( \sigma_i = (i = x, y, z) \) is the pseudospin Pauli matrices, \( \lambda_{\text{so}} \) is the vertical distance between the sublattices A and B, and \( E_z \) is an electric field normal to the silicene sheet, see Fig. 1. Further, \( \lambda_{\text{so}} \) is the SOI strength and \( s_z = 1 \) for the up (down) electron spin. Inserting the factors \( \tau \) and \( \sigma_i \) in Eq. (1) gives the Hamiltonian \( H_z \) with the \((+/-)\) sign for the \( K (K') \) valley

\[
H_z = \left[ \begin{array}{cc} \lambda_z(s_z) & v_F \pi_x - \lambda_z(s_z) \\ -\lambda_z(s_z) & \pi_y \end{array} \right], \tag{2}
\]

where \( \lambda_z(s_z) = \pm \lambda_{\text{so}} s_z + \ell E_z \) and \( \pi_x = \pi_x \pm i \pi_y \). Using the gauge \( A_y = -By \) and the ansatz \( \Psi(x, y) = \exp(i k x) \psi(y) / \sqrt{L_y} \), with \( L_x \) the system’s length in the \( x \) direction, leads to the eigenvalues

\[
E_{n_x n_y}^{+} = p h \omega_c \left( n + |\lambda_z(s_z)|^2 \right)^{1/2}. \tag{3}
\]

Here, \( p = +1(-1) \) labels the electron (hole) states, \( n \geq 1 \) is the LL index, \( \lambda_z = \lambda_{\text{so}} / \hbar \omega_c, \omega_c = \sqrt{2 eB / \hbar} \), and \( l_B = \sqrt{\hbar / eB} \). Note that the energy does not depend on \( k_x \). Setting \( s_z = y / l_B - l_B k_y \), the associated spatial eigenfunctions of an electron near the \( K \) point are

\[
\psi_{n}^{+}(\xi) = \left( \eta_{1}^{+} \phi_{n}(\xi) \quad \eta_{2}^{+} \phi_{n-1}(\xi) \right), \tag{4}
\]

FIG. 1. Buckled honeycomb lattice of silicene. The two sublattices, formed by the blue and red atoms, are vertically separated by a distance \( 2t_c \).
with \( \phi_n \) the normalized Harmonic oscillator function and

\[
\eta^+_1 = \left[ \frac{\lambda_+(s_z) + E_{n,s,p}^+}{2E_{n,s,p}^+} \right]^{1/2}, \quad \eta^-_2 = -\frac{1}{p} \left[ E_{n,s,p}^+ - \lambda_+(s_z) \right]^{1/2}.
\]

(5)

For an electron near the \( K' \) valley, the results are similar. For \( n = 0 \), each valley involves only one solution with energy \( E_{0,s,z}^+ = \pm \hbar \omega_0 \lambda_+ (s_z) \) and eigenfunctions \( \psi_0^+ = [\phi_0(\xi),0]^T \). The electron energies at the \( K \) and \( K' \) valleys are related by \( E_{n,s,z}^+ = E_{n,-s,z}^+ \) for \( n \geq 1 \), and \( E_{0,-s,z}^- = -E_{0,s,z}^- \) for \( n = 0 \).

**Modulated silicene.** We now assess the influence of an external periodic potential and/or that of a modulated field \( E_z \). As in the case of a 2DEG \(^{10,11}\) or graphene, \(^{12}\) the main effect of either modulation is to broaden the LLs into energy bands that oscillate with \( B \) and \( k_y \). Each LL though splits into four branches, two for the valley and two for the spin degree of freedom due to the SOI.

(i) Potential modulation. We consider a periodic potential \( V(y) = V_0 \cos(Cy) \), \( C = \pi / a_0 \), with \( a_0 \) its period, added to \( H \) as \( V(y)I \), with \( I \) is the identity matrix. For small \( V_0 \), we can use first-order perturbation theory to find the correction to the eigenvalues (3). For an electron near the \( K \) and \( K' \) valleys, the correction is

\[
\Delta E_{n,s,z}^\pm (k_y) = V_0 \cos(Cy) e^{-u^2/2} G_{n,s,p}^\pm,
\]

(6)

\[
G_{n,s,p}^+ = |\eta_1^+|^2 L_n(u) + |\eta_2^+|^2 L_{n-1}(u),
\]

(7)

\[
G_{n,s,p}^- = |\eta_1^+|^2 L_{n-1}(u) + |\eta_2^+|^2 L_n(u),
\]

(8)

where \( u = C^2 k_y^2 / 2, x_0 = \frac{L_x}{2} k_y \), and \( L_n(u) \) are the Laguerre polynomials. The energy correction depends on the wave vector \( k_y \) through \( x_0 \). That is, the periodic potential broadens the discrete LLs into bands. Given that the polynomials \( L_n(u) \) oscillate for large \( n \), in addition to the function \( \cos(Cy) \), one easily sees that the bandwidths (6) oscillate with the magnetic field \( B \). For \( n = 0 \), the energy correction is

\[
\Delta E_{0,s,z}^\pm (k_y) = V_0 \cos(Cy) e^{-u^2/2}.
\]

(9)

Note that the bandwidths (6) are different for spins up and down because of the spin-dependent coefficients \( \eta_{1,2}^\pm \).

(ii) Field modulation. We replace the field \( E_z \) in Eq. (1) by a periodic one \( E_z(y) = E_0 \cos(Dy) \) with \( D = 2\pi / b_0 \) and \( b_0 \) is the period. The energy correction is

\[
\Delta' E_{n,s,z}^\pm (k_y) = \langle n, s, p, k_y | E_z(y) | n, s, p, k_y \rangle,
\]

(10)

\[
= \ell E_0 \cos(Dx_0) e^{-u'^2/2} G_{n,s,p}^\pm,
\]

(11)

\[
G_{n,s,p}^+ = |\eta_1^+|^2 L_n(u') - |\eta_2^+|^2 L_{n-1}(u'),
\]

(12)

\[
G_{n,s,p}^- = |\eta_1^+|^2 L_{n-1}(u') - |\eta_2^+|^2 L_n(u'),
\]

(13)

where \( u' = D^2 k_y^2 / 2 \). For \( n = 0 \), we find

\[
\Delta' E_{0,s,z}^\pm (k_y) = \pm \ell E_0 \cos(Dx_0) e^{-u'^2/2}.
\]

(14)

In Fig. 2, we show the broadened LLs versus the magnetic field \( B \), for \( k_y = 10^4 \text{ m}^{-1} \), in the presence of a field modulation, with \( b_0 = 300 \text{ nm} \) and \( \ell E_0 = 1 \text{ meV} \). We used the strength of the SOI \( \Delta \zeta = 3.9 \text{ meV} \) and the Fermi velocity \( v_F = 5.42 \times 10^5 \text{ m/s} \). The LLs resulting only from the potential modulation, with \( a_0 = 300 \text{ nm} \) and \( V_0 = 1 \text{ meV} \), are shown in the inset. As seen, the oscillatory \( E_z \) and \( V \) lift the spin and valley degeneracy of the LLs. Each LL \( (n \geq 1) \) splits into four branches except for certain values of \( B \) at which \( \cos(Dx_0) = 0 \) and the bandwidth vanishes. That occurs at fields \( B = B_c/(2m + 1) \), with \( B_c = 2(h/e)k_x/\pi b_0 \) and \( m \) is a nonnegative integer. Notice that the \( n = 0 \) LL splits into two valley branches with the same spin as can be seen from \( E_{0,s,z}^+ = \pm \hbar \omega_0 \lambda (s_z) + \Delta' E_{0,s,z}^\pm \). For positive energies, this is the down spin.

The lifting of the spin and valley degeneracy results from the fact that for \( \ell E_0 = 0 \) the eigenvalues (3) are spin and valley degenerate, \( E_{n,s,z=\pm 1,p} = E_{n,s,z=\mp 1,p} = \hbar \omega_0 (n + \frac{1}{2}) \). But the eigenfunctions are not since the coefficients \( \eta_{1,2}^\pm \) are spin dependent, e.g., \( |\eta_1^+|^2 |_{s_z=\pm 1} = |\eta_2^+|^2 |_{s_z=\pm 1} = [\mp \omega_0 + E_{n,s,z=\pm 1,p}] / 2E_{n,s,p} \).

Then, all energy corrections depend on the spin.

At very low fields \( B \) the function \( \cos(Dx_0) \) in Eq. (6) fluctuates rapidly but the function \( e^{-u'^2/2} \) drastically reduces the oscillation amplitude. The same holds for the function \( \cos(Dx_0) \). Once \( B_c \) is attained, the energies increase monotonically and the bandwidth ceases to oscillate. This explains the form of the \( n = 0 \) LL.

The dc diffusive conductivity is given by

\[
\sigma_{\parallel \parallel} = \frac{e^2 c}{S} \sum_i \tau_0 \delta f_i (1 - f_i) v_{c i} v_{\mu i},
\]

(15)

where \( \tau_0 \) is the momentum relaxation time and \( v_{c i} \) and \( v_{\mu i} \) are the diagonal matrix elements of the velocity operator. Further, \( f_i = [1 + \exp(\beta (E_i - E_F))]^{-1} \) is the Fermi-Dirac function with \( \beta = 1/k_B T \) and \( T \) is the temperature. We focus here on the large-amplitude oscillations described by Eq. (12) and neglect the small-amplitude ones described by the collisional contribution. \(^{11}\)
Regarding the Hall conductivity $\sigma_{\mu\nu}^{nd}$, one can cast the form used in Ref. 11 in the familiar one

$$\sigma_{\mu\nu}^{nd} = \frac{i\hbar e^2}{S} \sum_{\nu' \neq \nu} \frac{\langle f_{\nu'} - f_{\nu} \rangle}{\langle E_{\nu'} - E_{\nu} \rangle^2} v_{\nu \nu'} v_{\nu' \nu},$$

(16)

where $v_{\nu \nu'}$ and $v_{\nu' \nu}$ are the non-diagonal matrix elements of the velocity operator and $\mu, \nu = x, y$. The sum runs over all quantum numbers $|\zeta\rangle = |\lambda, k_x, k_y, s_z\rangle$, $|\zeta\rangle$. (ii) 1D periodic potential or $E_z$ modulation. The modulation broadens the LLs into bands, cf. Eq. (6), and this induces a group velocity, proportional to the LL bandwidth, that results in a diffusive conductivity. Then, the electron velocity in the $n$-th Landau band is given by

$$v_{x,n,s,p}(k_x) = -(V_0C_0^2/\hbar)\sin(C_0) e^{-u/2}G_{n,s,p}^\pm(u),$$

(17)

and that due to a field modulation, $v_{x,n,s,p}^\pm$, by Eq. (14) with $V_0, u, C,$ and $G$ replaced by $\ell E_0, u', D,$ and $G'$, respectively. When the temperature is sufficiently low, the relaxation time can be evaluated at the Fermi energy, $\tau_F \approx \tau_F$. For a weak modulation, one can neglect\(^1^2\) the $k_x$ dependence of $f_z$. The result is

$$\sigma_{xx} = \frac{\hbar^2}{\hbar} \frac{\beta v_F^2}{\hbar} u e^{-u} \sum_{n,s,\pm} f_0(1 - f_0)(G_{n,s,p}^\pm)^2.$$  

(18)

For a field modulation, we obtain Eq. (15) with $V_0, u, C$, and $G$ replaced by $\ell E_0, u', D$, and $G'$, respectively.

Figure 3 shows the diffusive conductivity in the presence of only a field modulation. The solid (dashed) curve is the up (down) spin contribution. The oscillations are considerably spin resolved and at certain ranges of the field $B$ (coloured areas) a nearly 100% spin-polarized current is obtained. The two valleys make nearly the same contribution, i.e., no valley-resolved current is achieved because $|v_{x,n}^\pm| = |v_{x,n}^\mp|$. If only the $V(y)$ modulation is present ($|v_{x,n}^\pm| = |v_{x,n}^\mp|$), no sizable valley or spin gap is created in the oscillations, see the inset in Fig. 3. However, the oscillation amplitude is about 60 times larger than that of the field modulation because $|G_{n,s,p}^\pm| \gg |G_{n,s,p}^\pm|$. Notice that $\sigma_{xx} \approx 0$ for $0.7 T < B < 0.8 T$.

(iv) Potential and field modulations. To avoid the drawbacks of a single modulation and further ass the influence of parameters on the valley and spin splittings, we can combine the two modulations. To this end, we assume that a field modulation is already present, with fixed $E_0 = 1 \text{meV}/\ell$ and $a_0 = 300 \text{nm}$, and vary the strength $V_0$ and period $a_0$ of the potential modulation. We plot the valley polarization $p_v = (\sigma_+ - \sigma_-)/(\sigma_+ + \sigma_-)$ as a function of the ratio $V_0/E_0$ for different magnetic fields $B$ in Fig. 4(a) and different periods $a_0$ in Fig. 4(b); the two valley conductivities $\sigma_+$ and $\sigma_-$ include both spins. For low $V_0$, the polarization $p_v$ is maximal, whereas for high $V_0$ it disappears. Moreover, $p_v$ is maximal when the two modulations have the same period. In Fig. 4(c), we plot $p_v$ and the spin polarization $\sigma_s$, defined in a similar way, as functions of the field $B$ for $V_0 = 0.2 \text{meV}$ and $a_0 = b_0$. As seen, the presence of both modulations leads to a sizable $p_v$ because the total velocity differs for the two valleys; that is $|v_{x,n}^\pm + v_{x,n}^\mp| \neq |v_{x,n}^\pm + v_{x,n}^\mp|$. Both $p_v$ and $\sigma_s$ oscillate nearly periodically with $B$ but their periods increase at high $B$, cf. Eqs. (6) and (9). In contrast to Fig. 3, the spin gap is smaller and decreases at low fields $B$ because the LL index $n$ near $E_F$ is large; thus $\lambda_\pm (s_z) \ll E_{n,s,n}^\pm$ which yields $|\eta_\pm| \approx |\eta_0^\pm| \approx 1/2$.

Hall conductivity $\sigma_{yx}$. It is given by Eq. (16) and its evaluation requires the velocity operator $\hat{v} = \nabla_x H$, which for the two valleys is given by $\hat{v}^\pm = v_F(\hat{\sigma}_x \hat{e}_x + \hat{\sigma}_z \hat{e}_z)$. All its matrix elements, evaluated analytically, are diagonal in $k_x$ ($\delta_{k_x,k_y}$). To better understand the effect of the field $E_z$ modulation on $\sigma_{yx}$, we also consider a constant field $E_z$ that leads to $k_x$-independent LLs. Now a periodic, weak field $E_z$ perturbs the states $|\zeta\rangle^0$ and the new ones $|\zeta\rangle$ can be

![FIG. 3. Spin-up (solid curve) and spin-down (dashed curve) contributions to the diffusive conductivity, in units of $\sigma_0 = (e^2/\hbar)\ell \langle E \rangle^2 / \hbar$, versus the field $B$, when only the field modulation is present with $E_0 = 1 \text{meV}/\ell$, $a_0 = 300 \text{nm}$, $T = 3 \text{K}$, and $n_0 = 5 \times 10^{11} \text{cm}^{-2}$. In the coloured regions, the conductivity is nearly spin polarized and the colour is that of the dominant spin state. The inset shows results only for a potential modulation with $V_0 = 1 \text{meV}$, $a_0 = 300 \text{nm}$, and the same $T$ and $n_0$. Note the increase in the oscillation amplitude.](image1)

![FIG. 4. (a) Valley polarization $p_v$ versus the ratio $V_0/E_0$ for different fields $B$. The parameters are $E_0 = 1 \text{meV}/\ell$, $b_0 = a_0 = 300 \text{nm}$, $T = 3 \text{K}$, and $n_0 = 5 \times 10^{11} \text{cm}^{-2}$. (b) The same as in (a) but for different periods $a_0$ at $B = 0.6 \text{T}$. $p_v$ is maximal for low strengths $V_0$ and $a_0 = b_0$. (c) Valley (solid curve) and spin (dotted curve) polarizations versus magnetic field $B$ for $V_0 = 0.2 \text{meV}$ and $a_0 = b_0 = 300 \text{nm}$.](image2)
Figure 5 shows the Hall conductivity versus the field $B$ replaced by a series of short plateaux and steps (solid curve). LL valley splitting is comparable to their spin splitting, see due to spin resolution. However, for a modulated field, the modulation does very weak, hence the extra plateaux are mostly weak, and (ii) they also are nearly periodic in the field $B$, phase-shifted by $\pi$, and their periods increase with $B$.

We also studied the Hall conductivity $\sigma_{yx}$ and showed that the field modulation creates extra narrow plateaux within the standard, integer-$n$ LL plateaux. All of them are due to sharp changes in $E_F$, as it moves through the LLs, and the new ones result from the lifting of the spin and valley degeneracies and the corresponding transitions between the four ($n \geq 1$) or two ($n = 0$) sublevels. The step structure, within an integer-$n$ LL plateau, replaces the latter by a series of narrow plateaux and steps.

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