Transport in two-dimensional materials

Vassilios Vargiamidis
WCPM, University of Warwick, UK
Outline

Overview of graphene

- Crystal structure, band structure, Dirac cones, etc.
- Density of states

Transport in silicene

- Tuning the charge conductance and transport gap
- Spin-resolved, valley-resolved, and charge conductances
- Near perfect spin and valley polarizations
- Topological phase transitions

Possible applications

Summary
Overview of graphene
Graphene pioneers (Nobel prize 2010)

New 2D electron system (Manchester 2004)
Nanoscale electron system with *tunable properties*;
Field-effect enabled by gating: tunable carrier density

1. very high mobilities in its suspended form: \( \mu \sim 200.000 \text{cm}^2/(\text{V.s}) \)
2. ballistic transport over sub-micron distances: \( l \sim 1 \mu \text{m} \)
3. high thermal conductivity: \( \kappa = 5000 \text{W}/(\text{m.K}) \),
4. chemically stable, very stiff, . . .
Semimetal (zero bandgap): electrons and holes coexist

- Electronic energy dispersion: Dirac points
- Hexagonal BZ: 2 inequivalent points $K$ and $K'$ where carriers mimic relativistic massless Dirac particles
- Linear energy dispersion at $K$ and $K'$: massless Dirac fermion model in 2D

\[ E = \sqrt{m^2 c^4 + p^2 c^2}, \quad m \to 0 \]

\[ v_F = 10^6 \text{ m/s} = \frac{c}{300} \]

Slow, but ultrarelativistic Dirac Fermions!
Graphene allotropes

2D Graphene: presumed not to exist in the free state (2004)

3D Graphite

1D Carbon Nanotube (1991) (rolled-up cylinder of graphene)

0D Fullerenes (“buckyball”) (1985)
Graphene’s honeycomb lattice

1\textsuperscript{st} Brillouin zone

Unit cell

\[ \vec{\alpha}_1 = \frac{\alpha}{2} (\sqrt{3}, 3) \]
\[ \vec{\alpha}_2 = \frac{\alpha}{2} (-\sqrt{3}, 3) \]

\[ \vec{K}_1 = \frac{2\pi}{3\alpha} (\sqrt{3}, 1) \]
\[ \vec{K}_2 = \frac{2\pi}{3\alpha} (-\sqrt{3}, 1) \]

\( \alpha = 0.142 \text{ nm} \)

Inequivalent points \( \vec{K} \) and \( \vec{K}' \)
Tight-binding model for electrons on the honeycomb lattice

\[ H = \sum_k \left( a_k^\dagger b_k^\dagger \right) h_k \left( a_k b_k \right) \]

\[ h_k = \begin{pmatrix} 0 & f(k) \\ f^*(k) & 0 \end{pmatrix} \]

\[ f(k) = 1 + e^{-ik \cdot a_1} + e^{-ik \cdot a_2} \]

Dirac points at K and K’

Energy bands:

\[ \varepsilon_k^\lambda = \lambda t \sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2} k_x a \right) \cos\left(\frac{3}{2} k_y a \right) + 4\cos^2\left(\frac{\sqrt{3}}{2} k_x a \right)} \]

\[ \lambda = \pm 1: \text{band index} \quad t \approx -3 \text{ eV} \]

Semi-metal
Dirac points

The Dirac points are situated at the points $\mathbf{k}^D$ where

$$\varepsilon^D_{\mathbf{k}} = 0$$

Time-reversal symmetry: $\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}}$

Dirac points occur in pairs:

twofold valley degeneracy
Low-energy regime of the TB model: 2D Dirac equation

\[ H_{q}^{\xi} = \xi \hbar \nu_{F} \begin{pmatrix} 0 & q_{x} - i q_{y} \\ q_{x} + i q_{y} & 0 \end{pmatrix} = \xi \hbar \nu_{F} \mathbf{q} \cdot \mathbf{\sigma} \]

\( \xi = \pm 1 \) Valley pseudospin for K and K’ points

\( \mathbf{\sigma} = \sigma_{x} \hat{i} + \sigma_{y} \hat{j} \) Pauli matrices of the sublattice pseudospin

\[ \epsilon_{q,\xi}^{\lambda} = \lambda \hbar \nu_{F} |\mathbf{q}| \]

\[ \nu_{F} = \frac{3|t|a}{2\hbar} \approx 8.7 \times 10^{5} \text{m/s} \]
Transport in silicene
Crystal structure of silicene

- A potential difference $\propto 2\ell E_z$ arises between silicon atoms at A sites and B sites when an electric field $E_z$ is applied.
- Energy gap 1.55 meV
- Silicene is compatible with silicon-based technology

$\lambda_{so} \approx 3.9 \text{meV}$

Buckled structure

$2\ell = 0.46 \text{Å}$
Low-energy Hamiltonian

\[ H_{z} = \hbar \nu_{F} (\tau_{x} k_{x} - \xi \tau_{y} k_{y}) - \xi s_{z} \lambda_{so} \tau_{z} + \Delta_{z} \tau_{z} \]

\( \xi = \pm 1 \) valley index \( \quad \nu_{F} \approx 5 \times 10^{5} \text{ m/s} \) Fermi velocity

\( \tau_{i} \) Pauli matrices of sublattice pseudospin

\( \Delta_{z} = e \ell E_{z}, \quad E_{z} \) electric field

\( s_{z} \) electron spin operator normal to silicene plane \( (s_{z} = \pm 1) \)

\( \lambda_{so} \approx 3.9meV \) spin-orbit interaction

Eigenfunctions

\[ \Psi_{\lambda,k,\xi,s_{z}}(\vec{r}) = \frac{1}{\sqrt{2S}} \left( \frac{\sqrt{1 + \lambda \cos \theta}}{\lambda \sqrt{1 - \lambda \cos \theta} e^{i \xi k_{z}}} \right) e^{i \vec{k} \cdot \vec{r}} \]

Eigenvalues

\[ E_{\lambda,k,\xi,s_{z}} = \lambda \sqrt{\hbar^{2} \nu_{F}^{2} k^{2} + (\Delta_{z} - \xi s_{z} \lambda_{so})^{2}} \]

\( \lambda = +1(-1) \) electron (hole) states
Band structure

\[ \delta_z = \frac{\Delta_z}{\lambda_{so}} \]
\[ \beta = \frac{\hbar v_F k}{\lambda_{so}} \]

\[ \delta_z = 1 \iff E_z = 0.17 V/nm \]
Density of states

\[
D(E) = \frac{|E|}{\pi \hbar^2 v_F^2} \left[ \Theta(|E| - |\Delta_z - \lambda_{so}|) + \Theta(|E| - |\Delta_z + \lambda_{so}|) \right]
\]

The DOS reflects the two gaps that open in the system.

Evolution of the gap $\delta$ with the electric field:

\[
\delta = 2 \lambda_{so} |\delta_z - \xi s_z|
\]

The gap closes when $\delta_z = \xi s_z = \pm 1$

This yields $E_z = \xi s_z E_c$ with

\[
E_c = \lambda_{so} / \ell = 17 \text{ meV/Å}
\]
Spin- and valley-polarized transport across ferromagnetic (FM) silicene junctions
Low-energy Hamiltonian

\[ H_{\xi} = \nu_F \left( \tau_x p_x - \xi \tau_y p_y \right) + \Delta_{\xi z} \tau_z + U - s_z M \]

with \( \Delta_{\xi z} = \Delta_z - \xi s_z \lambda_{so} \)

Barrier potential (gate voltage)

Exchange field

Single FM junction

\[ U, M \]

Eigenfunctions

\[ \Psi_I(\vec{r}) = A \begin{pmatrix} c_F e^{i\xi \theta} \\ E_N \end{pmatrix} e^{i\vec{k} \cdot \vec{r}} + r A \begin{pmatrix} -c_F e^{-i\xi \theta} \\ E_N \end{pmatrix} e^{i(-k_x x + k_y y)} \]

\[ \Psi_{II}(\vec{r}) = a \begin{pmatrix} c'_F e^{i\xi \phi} \\ \varepsilon_F \end{pmatrix} e^{i\vec{k'} \cdot \vec{r}} + b \begin{pmatrix} -c'_F e^{-i\xi \phi} \\ \varepsilon_F \end{pmatrix} e^{i(-k'_x x + k'_y y)} \]

\[ \Psi_{III}(\vec{r}) = t A \begin{pmatrix} c_F e^{i\xi \theta} \\ E_N \end{pmatrix} e^{i\vec{k} \cdot \vec{r}}, \quad A = 1/\sqrt{2E_F E_N} \]

Transmission amplitude

\[ c_F = \hbar \nu_F k_F, \quad E_N = E_F + \xi s_z \lambda_{so}, \quad \varepsilon_F = E_F - U + s_z M - \Delta_{\xi z} \]
Transmission and conductance through a FM junction

Incidence at an angle $\theta$:

$$T_{\xi_z}(\theta) = \frac{\cos^2 \theta \cos^2 \phi}{\cos^2 (k'_x d) \cos^2 \theta \cos^2 \phi + \sin^2 (k'_x d)(\alpha + \alpha^{-1} - 2 \sin \theta \sin \phi)^2 / 4}$$

with $\alpha = \varepsilon_F k_F / E_N k'_F$ and $k'_x = \sqrt{k'_F^2 - k_F^2 \sin^2 \theta}$

Fermi wave vectors:

$$k_F = \frac{\sqrt{E_F^2 - \lambda_{so}^2}}{\hbar \nu_F}$$

$$k'_F = \frac{\sqrt{(E_F - U + s_z M)^2 - \Delta_{\xi_z}^2}}{\hbar \nu_F}$$

$T_{\xi_z}(\theta) = 1$ for $k'_x d = n\pi$ as in graphene

Normal incidence $\theta = 0$:

$$T_{\xi_z}(0) = \frac{1}{1 + \sin^2 (k'_x d)(\alpha - \alpha^{-1})^2 / 4}$$

Conductance:

$$G_{\xi_z} = G_0 \int_{-\pi/2}^{\pi/2} T_{\xi_z}(\theta) \cos \theta d\theta = G_0 g_{\xi_z}$$

$$G_0 = e^2 k_F W / 2\pi h$$

$W$ sample width
Spin-resolved conductance

Resonances for high barrier or deep well with amplitude between 2/3 and 1

Transport at the Dirac point (DP) is due to evanescent modes

Transport via evanescent modes is suppressed with increasing $\delta_z$ and the dip develops to transport gap

$\delta_z = 0 \quad m = M / E_F = 0$

$$g_{\uparrow(\downarrow)} = \frac{g_{K\uparrow(\downarrow)} + g_{K\uparrow(\downarrow)}}{2}$$

$E_F = 40 meV, \quad d = 110 nm$
Tuning the conductance

\[ \delta_z = \Delta_z / \lambda_{so} = 11.9 \]

For the Fermi level lies in the gap

\[ g_c = g_\uparrow + g_\downarrow \]

\[ U / E_F = 2, \ M = 2.5\text{meV} \]

\[ k'_x = \sqrt{k'_F^2 - k_F^2 \sin^2 \theta} \]

\[ \Delta'_z = \xi \Delta_{so} \pm |E_F - U + s_z M| \]

No analog in graphene

In graphene \( \Delta_{\xi z} = 0 \)

\[ \Rightarrow k'_F = \left| E_F - U \right| / \hbar \nu_F \]

It cannot be made imaginary

For \( \Delta_z > \Delta'_z \) the Fermi level lies in the gap

The junction acts as an electric switch
Current is entirely carried by spin-down electrons at the $K'$ ($g_\downarrow$ oscillatory).

Only evanescent modes contribute to $g_\uparrow$ (monotonically decreasing behavior)\[^2\]
Near the DP $k_F'$ is imaginary

As $\delta_z$ increases the evanescent modes are gradually damped out $\Rightarrow$ transport gap

$\varepsilon_{s}^{(1,2)} = \frac{E_F^{c(1,2)}}{\lambda_{so}}$

Transport gap when $E_F < E_F^c$

$E_F^c = \Delta_z - \lambda_{so}$
We aim now to explore possible spin and valley polarizations in FM silicene
Spin-resolved and charge conductances

\[ m = M / E_F \]

Relative shift of \( g_\uparrow \) and \( g_\downarrow \) in the presence of \( M \)

Transport gaps for both

\[ g_c \text{ is periodic function of } U/E_F \]

\[ T_u = \pi \hbar \nu_F / E_F d\delta_\lambda = 0.235 \]

for \( |U/E_F| >> 1 \)
Valley-resolved and charge conductances

\[ g_{K(K')} = \frac{g_{K(K')}^\uparrow + g_{K(K')}^\downarrow}{2} \]

Splitting of the peaks of \( g_c \) with \( m \)

Splitting of the peaks of \( g_{K'} \) due to the broken valley symmetry in the presence of \( m \)
Spin polarization

\[ p_s = \frac{g_\uparrow - g_\downarrow}{g_\uparrow + g_\downarrow} \]

The range of \( p_s \approx 1 \) increases with \( \delta_z \) or \( m \)

For large \( \delta_z \) or \( m \):

- only a single spin band contributes to the current
- the evanescent modes are suppressed
- the change of sign is due to the relative shift of \( g_\uparrow \) and \( g_\downarrow \)

Spin polarization can be inverted by changing \( U \)
Spin and valley polarization

$p_s = \frac{g_{\uparrow} - g_{\downarrow}}{g_{\uparrow} + g_{\downarrow}}$

$p_v = \frac{g_K - g_{K'}}{g_K + g_{K'}}$

$p_s$ and $p_v$ can be inverted by changing the direction of $M$

This is directly related to the relative shift of $g_{\uparrow}$ and $g_{\downarrow}$
Transition from a topological insulator to band insulator regime

Spin-Hall conductivity becomes zero for high $E_z$
The results for the polarized transport through a FM silicene junction can be used to realize silicene-based, high-efficiency spin- and valley-filter.

Other possible applications:

• In spintronics (due to longer spin-diffusion time and spin-coherence length)
• In quantum computing
• Silicene can overcome difficulties associated with potential applications of graphene in nanoelectronics (lack of a controllable gap)
• Optoelectronics
• Energy harvesting
Summary

• The buckled structure of silicene can facilitate *the control of its band gap* by the application of an electric field $E_z$.

• Above a critical $E_z$ the charge conductance $g_c$ through a silicene FM junction changes from an oscillatory to a monotonically decreasing function of the junction width $d$. A gap develops near the DP with increasing $E_z$.

• These features can be used for the realization of electric-field controlled switching.

• The spin $p_s$ and valley $p_v$ polarizations near the DP increase with $E_z$ or $M$, and become nearly perfect ($\approx 100\%$) above certain $E_z$ and $M$ values.

• $p_s$ and $p_v$ can be inverted by reversing the direction of $M$ or $U$: near perfect spin and valley filtering

*Most of the results* have no analog in graphene

*APL 105, 223105 (2014), JAP 117, 094305 (2015)*