Transport in two-dimensional materials

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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

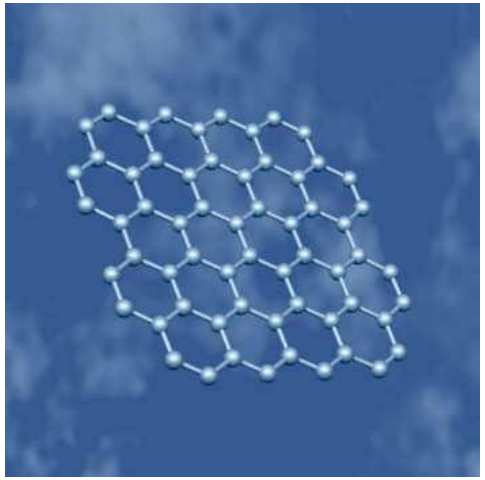
Summary

Overview of graphene

Graphene pioneers (Nobel prize 2010)

Andrey Geim

Kostya Novoselov



Philip Kim

New 2D electron system (Manchester 2004)

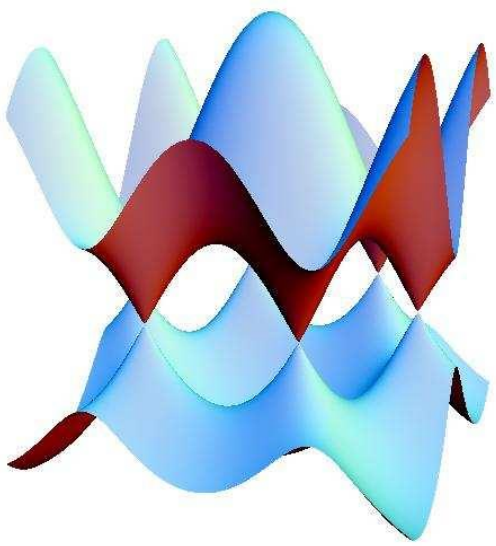
Nanoscale electron system with *tunable properties;*
Field-effect enabled by gating: tunable carrier density

1. very high mobilities in its suspended form: $\mu \sim 200.000 \mathrm{cm}^2/(\mathrm{V.s})$
2. ballistic transport over sub-micron distances: $l \sim 1\mu m$
3. high thermal conductivity: κ=5000W/(m.K),
4. chemically stable, very stiff, . . .

Semimetal (zero bandgap): electrons and holes coexist

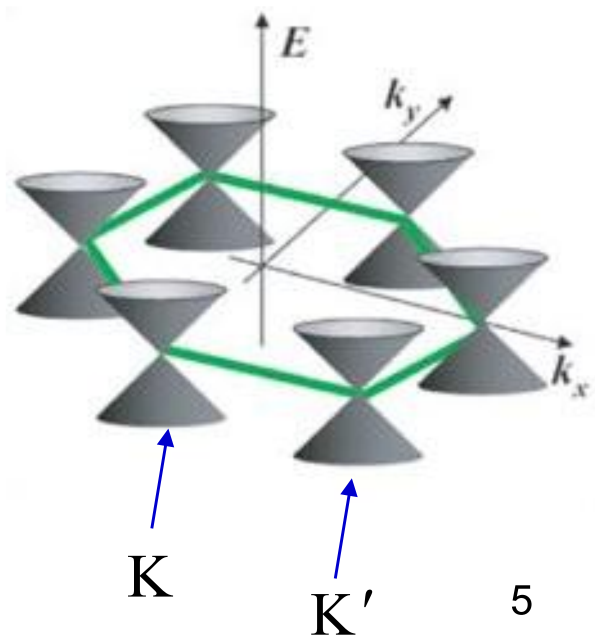
- Electronic energy dispersion: Dirac points
- Hexagonal BZ: 2 inequivalent points K and K′ where carriers mimic relativistic massless Dirac particles
- Linear energy dispersion at K and K′: massless Dirac fermion model in 2D

$$E = \sqrt{m^2c^4 + p^2c^2}, \qquad m \to 0$$



$$v_F = 10^6\,\mathrm{m/s} = \frac{c}{300}$$

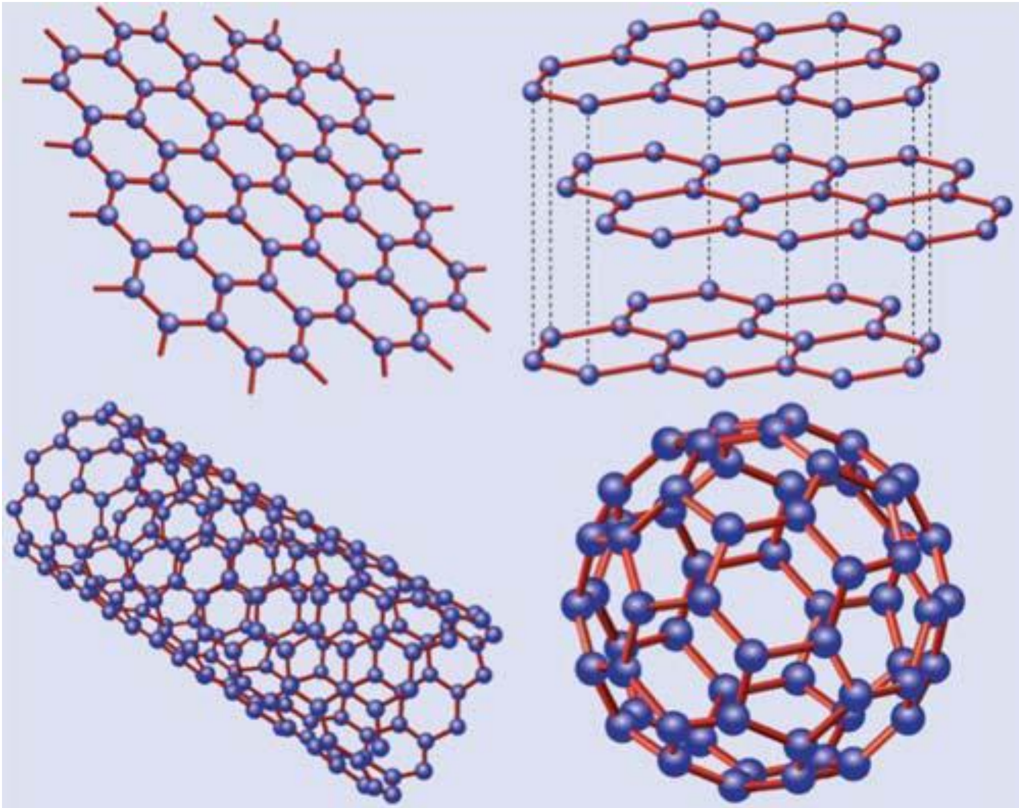
Slow, but ultrareletivistic Dirac Fermions!



Graphene allotropes

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

(2004)



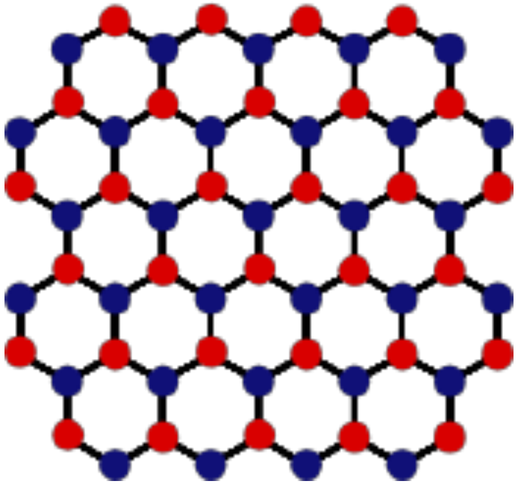
3D Graphite

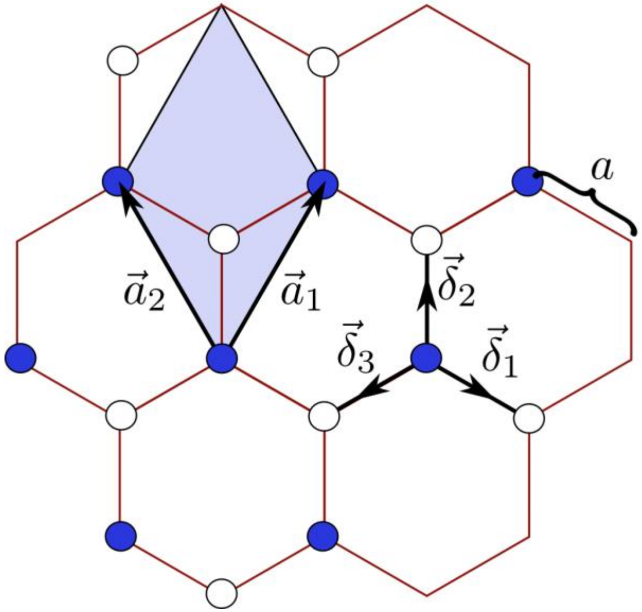
1D Carbon Nanotube (1991)
(rolled-up cylinder of graphene)

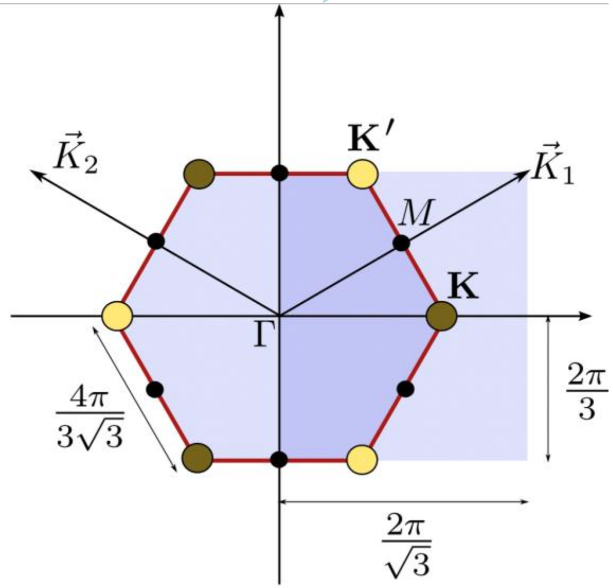
0D Fullerenes ("buckyball")
(1985)

Graphene's honeycomb lattice

1st Brillouin zone







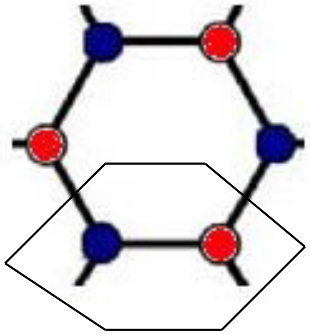
$$\vec{\alpha}_1 = \frac{\alpha}{2}(\sqrt{3}, 3)$$

$$\vec{\alpha}_2 = \frac{\alpha}{2}(-\sqrt{3}, 3)$$

$\boxed{\alpha = 0.142 \text{ nm}}$

$$\vec{K}_1 = \frac{2\pi}{3\alpha}(\sqrt{3}, 1)$$

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



Unit cell

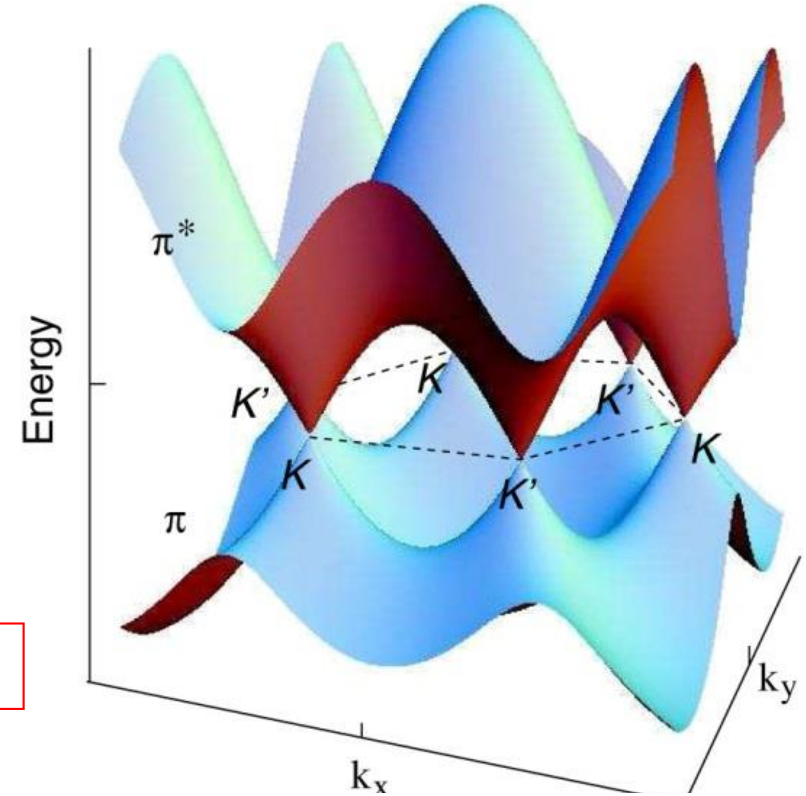
Inequivalent points $\vec{K}$ and $\vec{K'}$

Tight-binding model for electrons on the honeycomb lattice

$$H = \sum_{\mathbf{k}} (a_{\mathbf{k}}^\dagger \; b_{\mathbf{k}}^\dagger) \, h_{\mathbf{k}} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix}$$

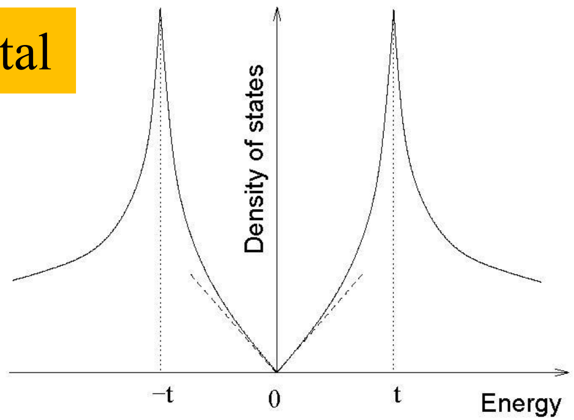
$$h_{\mathbf{k}} = \begin{pmatrix} 0 & f(\mathbf{k}) \\ f^*(\mathbf{k}) & 0 \end{pmatrix}$$

$$f(\mathbf{k}) = 1 + e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2}$$



Dirac points at K and K'

Semi-metal



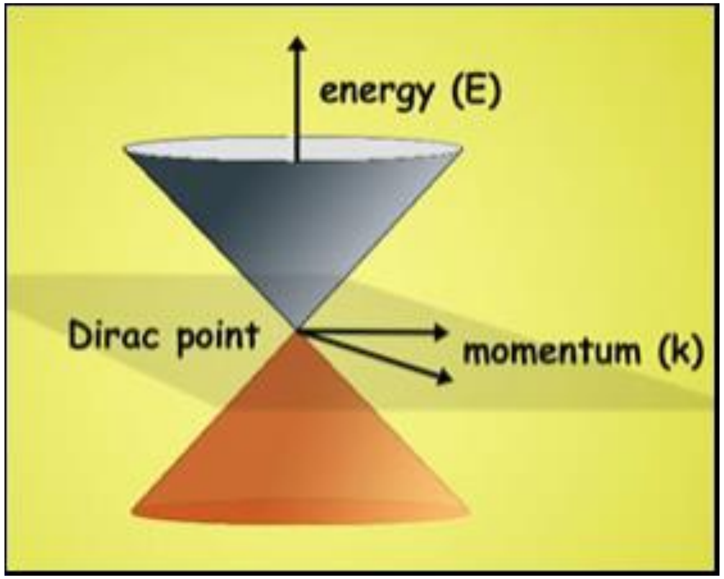
Energy bands:

$$\varepsilon_{\mathrm{k}}^{\lambda} = \lambda t \sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{3}{2}k_y a\right) + 4\cos^2\left(\frac{\sqrt{3}}{2}k_x a\right)}$$

$\lambda = \pm 1$: band index

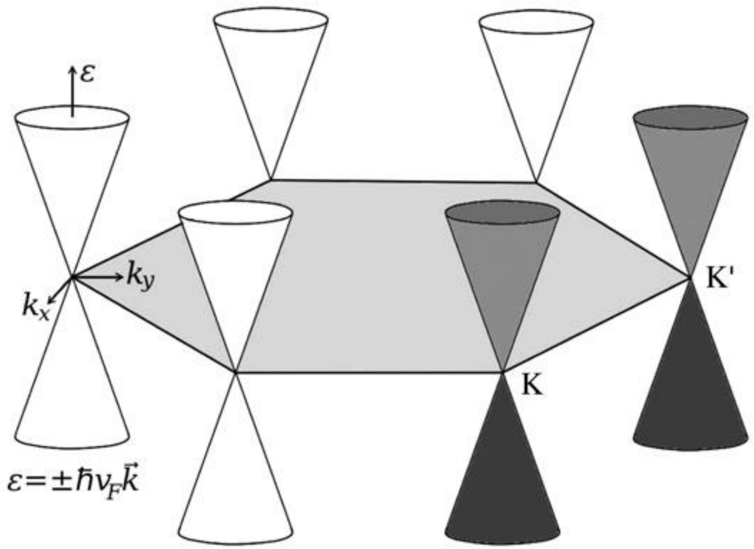
$$t \approx -3\,\mathrm{eV}$$

Dirac points



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

$$\boxed{\varepsilon^{D}_{\mathbf{k}} = 0}$$



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

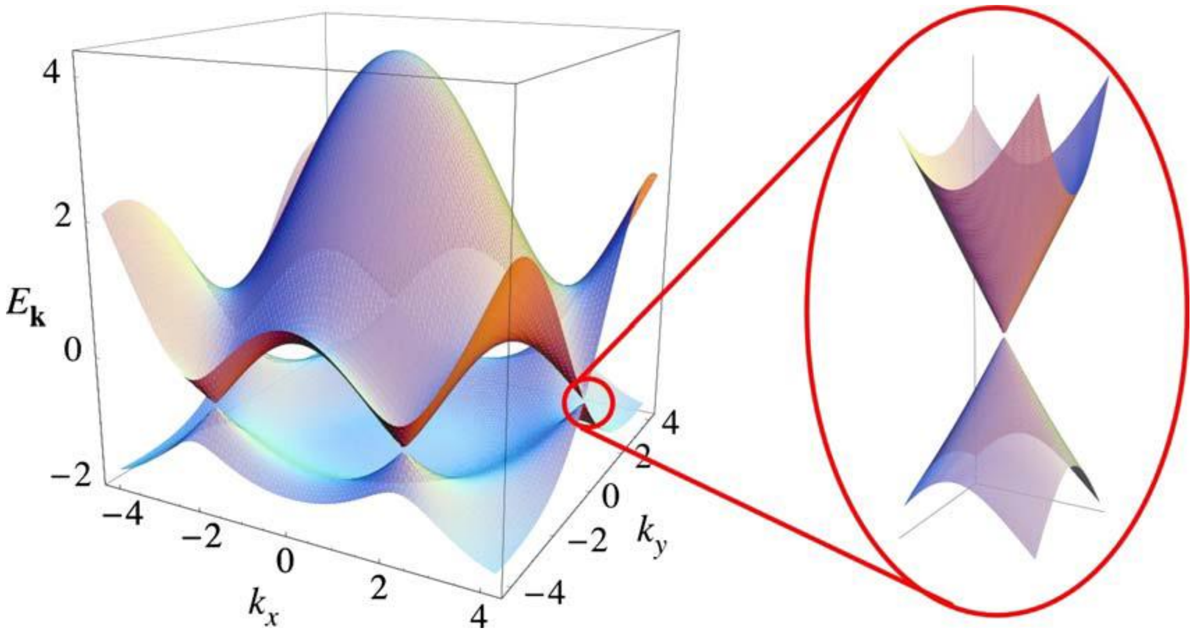
$$\mathrm{H}_{\mathbf{q}}^{\xi} = \xi\hbar\upsilon_{\mathrm{F}}\begin{pmatrix} 0 & \mathrm{q_x - iq_y} \\ \mathrm{q_x + iq_y} & 0 \end{pmatrix} = \xi\hbar\upsilon_{\mathrm{F}}\mathbf{q}\cdot\boldsymbol{\sigma}$$

$\xi = \pm 1$ Valley pseudospin for K and K' points

$\boldsymbol{\sigma} = \sigma_x\hat{\boldsymbol{\imath}} + \sigma_y\hat{\boldsymbol{\jmath}}$ Pauli matrices of the sublattice pseudospin

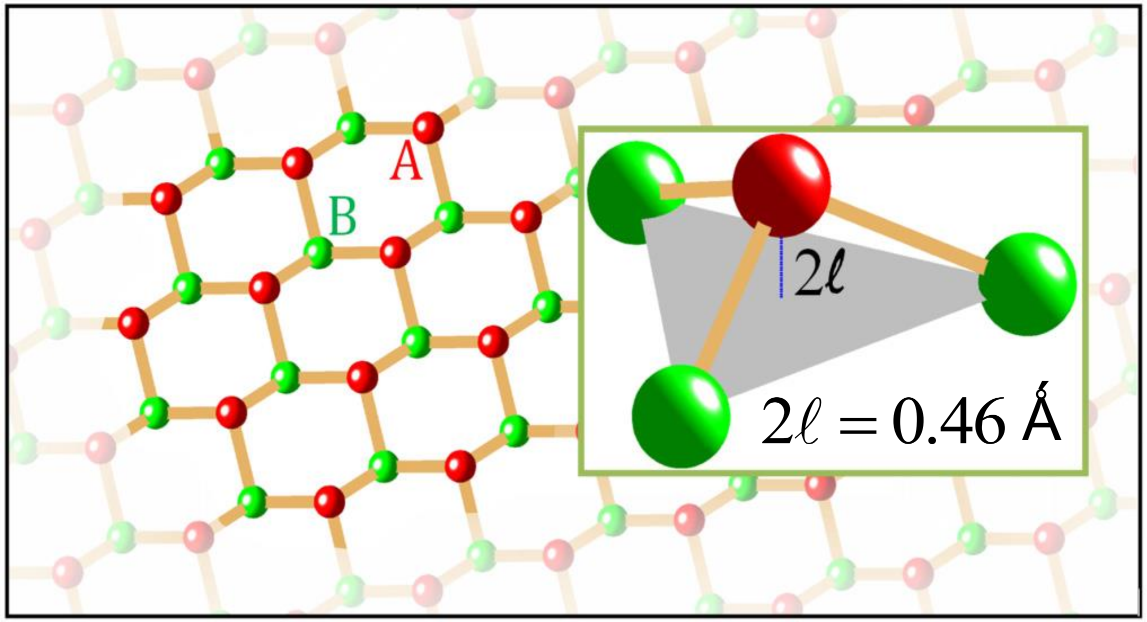
$$\varepsilon_{\boldsymbol{q},\xi}^{\lambda} = \lambda\hbar\upsilon_F|\boldsymbol{q}|$$

$$\upsilon_{\mathrm{F}} = \frac{3|\mathrm{t}|\mathrm{a}}{2\hbar} \approx 8.7\times10^{5}\mathrm{m/s}$$



Transport in silicene

Crystal structure of silicene



$\lambda_{so} \approx 3.9meV$

Buckled structure

- A potential difference $\boxed{\propto 2\ell E_z}$ 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

Low-energy Hamiltonian

$$\boxed{H_{\xi} = \hbar\upsilon_F\left(\tau_x k_x - \xi\tau_y k_y\right) - \xi s_z \lambda_{so}\tau_z + \Delta_z \tau_z}$$

$\xi = \pm 1$ valley index $\upsilon_F \approx 5\times 10^5 m/s$ Fermi velocity

τ_i Pauli matrices of sublattice pseudospin

$\Delta_z = e\ell E_z$, E_z electric field

s_z electron spin operator normal to silicene plane $(s_z = \pm 1)$

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

Eigenfunctions

$$\Psi_{\lambda,\vec{k},\xi,s_z}(\vec{r}) = \frac{1}{\sqrt{2S}}\begin{pmatrix} \sqrt{1+\lambda\cos\theta} \\ \lambda\sqrt{1-\lambda\cos\theta}\, e^{i\xi\phi_k} \end{pmatrix} e^{i\vec{k}\cdot\vec{r}}$$

Eigenvalues

$$E_{\lambda,k,\xi,s_z} = \lambda\sqrt{\hbar^2\upsilon_F^2 k^2 + (\Delta_z - \xi s_z\lambda_{so})^2}$$

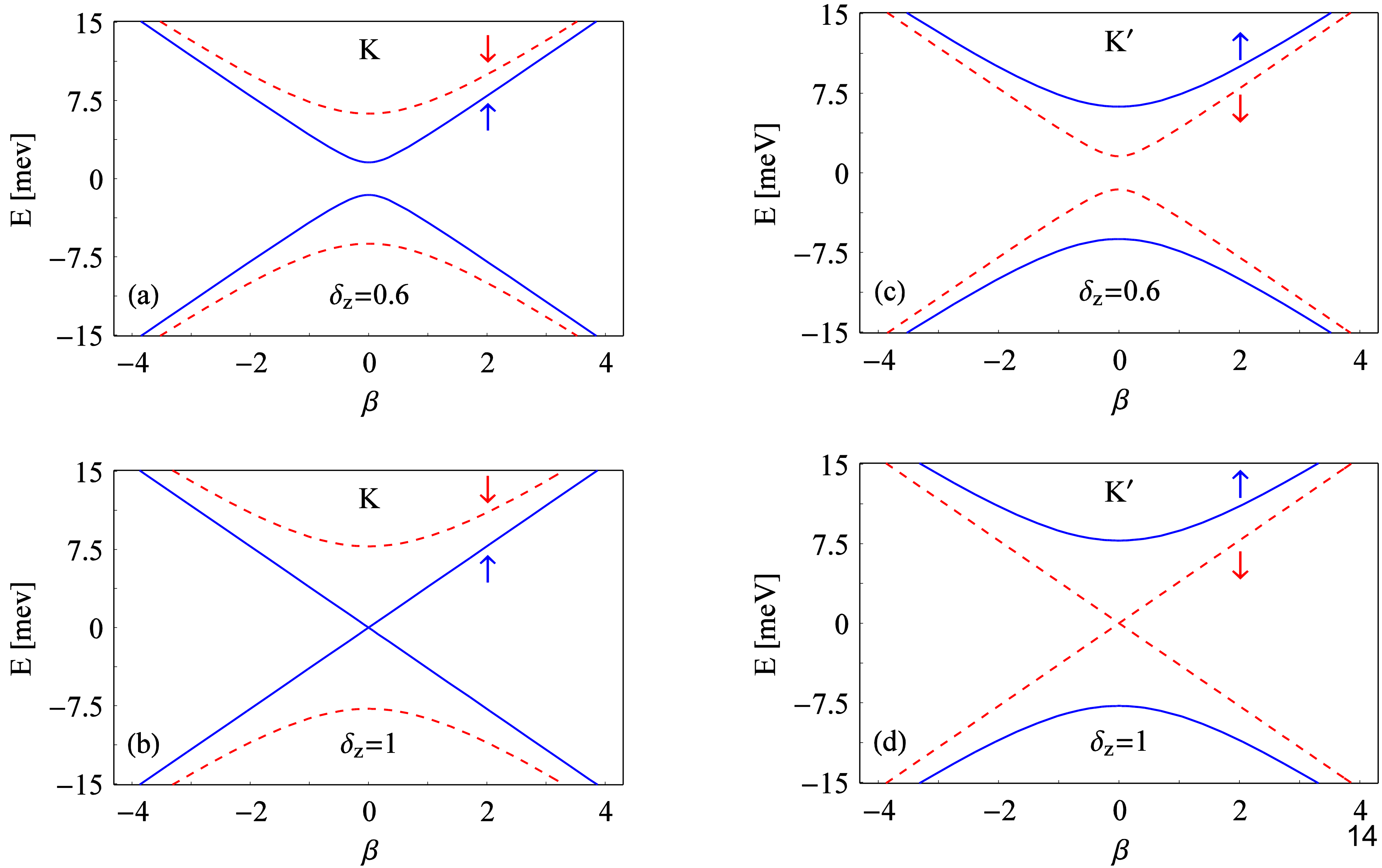
$\lambda = +1(-1)$ electron (hole) states

Band structure

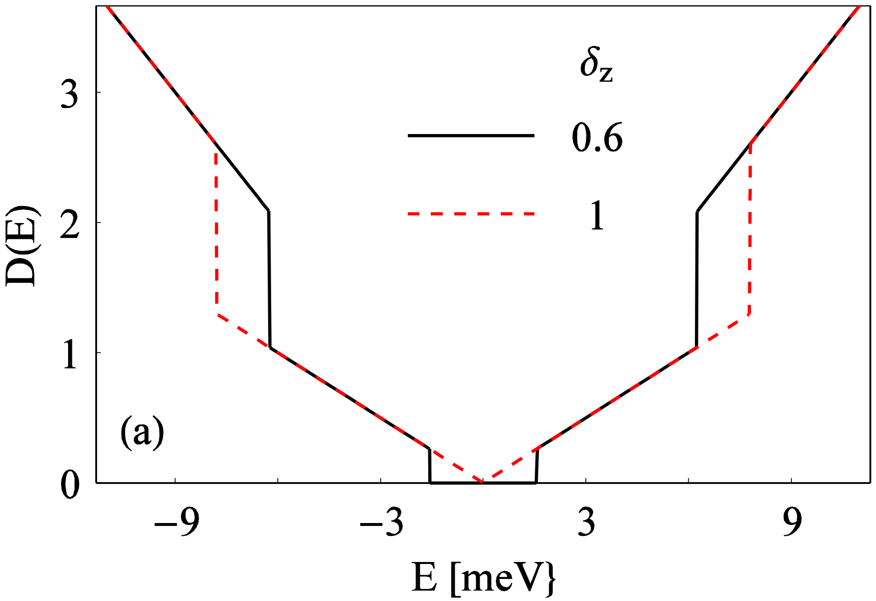
$\delta_z = \Delta_z / \lambda_{so}$

$\beta = \hbar \upsilon_F k / \lambda_{so}$

$\delta_z = 1 \Leftrightarrow E_z = 0.17 V / nm$

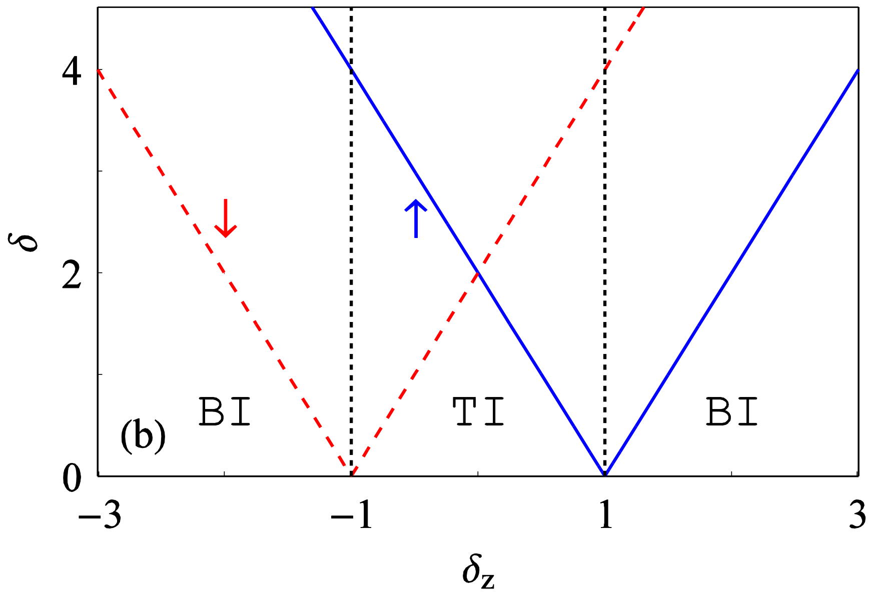


Density of states



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

The DOS reflects the two gaps that open in the system



Evolution of the gap δ 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

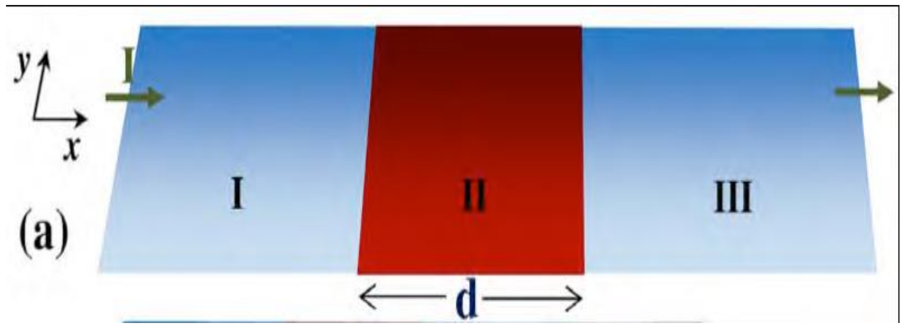
$$\boxed{H_\xi = \upsilon_F\left(\tau_x p_x - \xi\tau_y p_y\right) + \Delta_{\xi s_z}\tau_z + U - s_z M} \quad \text{with} \quad \Delta_{\xi s_z} = \Delta_z - \xi s_z \lambda_{so}$$

Barrier potential (gate voltage)

Exchange field

Single **FM** junction

U, M



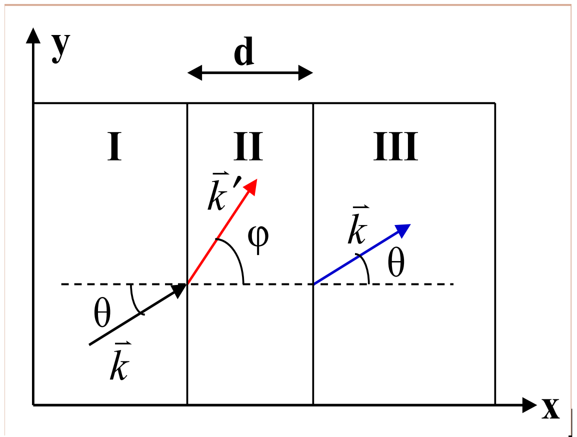
Eigenfunctions

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

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

$$\Psi_{III}(\vec{r}) = tA\begin{pmatrix} c_F e^{i\xi\theta} \\ E_N \end{pmatrix} e^{i\vec{k}\cdot\vec{r}}, \qquad A = 1\Big/\sqrt{2E_F E_N}$$

Transmission amplitude



$$c_F = \hbar\upsilon_F k_F\,, \quad E_N = E_F + \xi s_z \lambda_{so}\,, \quad \varepsilon_F = E_F - U + s_z M - \Delta_{\xi s_z}$$

Transmission and conductance through a FM junction

Incidence at an angle θ :

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

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

Fermi wave vectors:

$$k_F = \frac{\sqrt{E_F^2 - \lambda_{so}^2}}{\hbar\upsilon_F} \qquad k'_F = \frac{\sqrt{(E_F - U + s_z M)^2 - \Delta^2_{\xi s_z}}}{\hbar\upsilon_F}$$

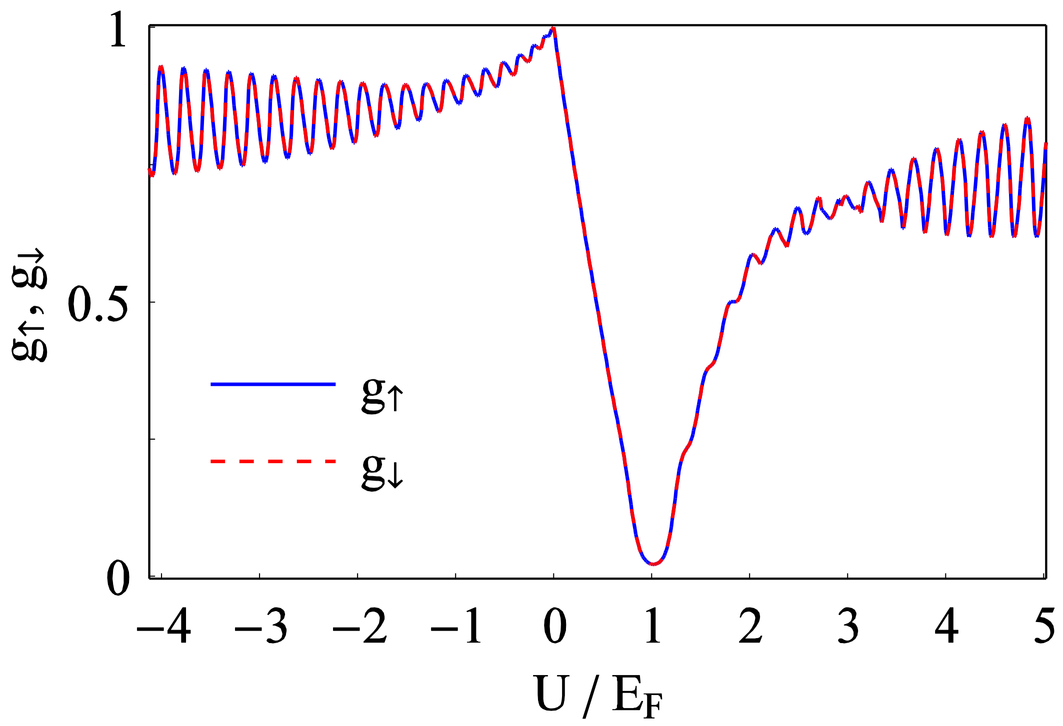
$\boxed{T_{\xi s_z}(\theta) = 1}$ for $k'_x d = n\pi$ as in graphene

Normal incidence $\theta = 0$: $T_{\xi s_z}(0) = \dfrac{1}{1+\sin^2(k'_x d)(\alpha-\alpha^{-1})^2/4}$ (in contrast to graphene it depends on barrier height)

Conductance: $G_{\xi s_z} = G_0 \int_{-\pi/2}^{\pi/2} T_{\xi s_z}(\theta)\cos\theta\, d\theta = G_0 g_{\xi s_z}$, $G_0 = e^2 k_F W / 2\pi h$

W sample width

Spin-resolved conductance



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

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

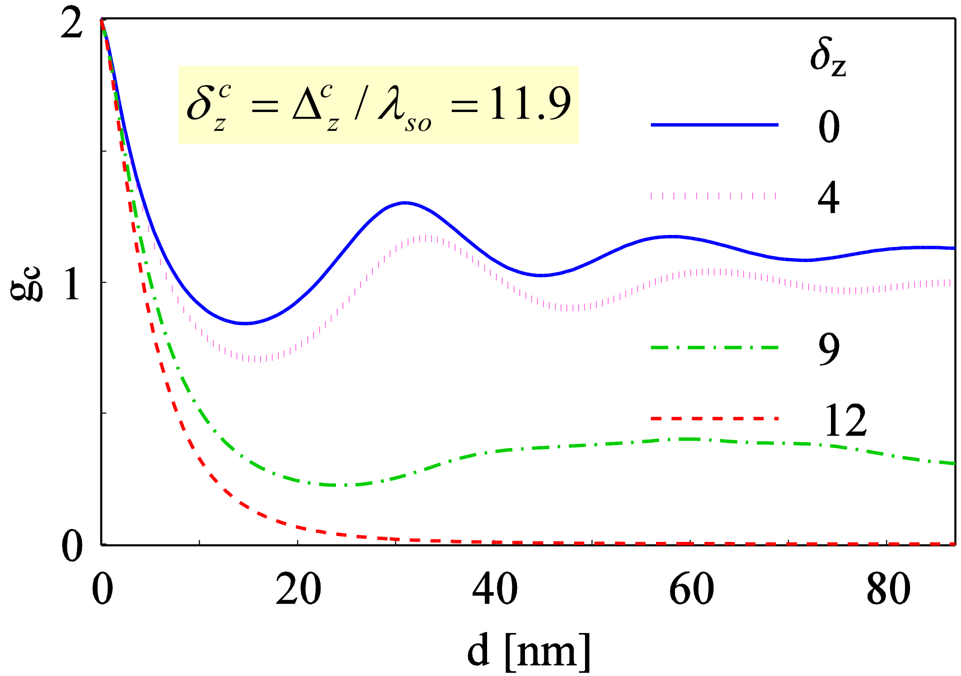
$$E_F = 40\,meV, \quad d = 110\,nm$$

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 δ_z and the dip develops to **transport gap**

Tuning the conductance



$$g_c = g_\uparrow + g_\downarrow$$

$$U / E_F = 2, \quad M = 2.5meV$$

$$k'_x = \sqrt{k_F'^2 - k_F^2 \sin^2\theta}$$

k'_x becomes imaginary when k'_F becomes imaginary

$$\Delta_z^c = \xi s_z \lambda_{so} \pm \left| E_F - U + s_z M \right|$$

No analog in graphene

In graphene $\Delta_{\xi s_z} = 0$

$$\Rightarrow k'_F = \left| E_F - U \right| / \hbar \upsilon_F$$

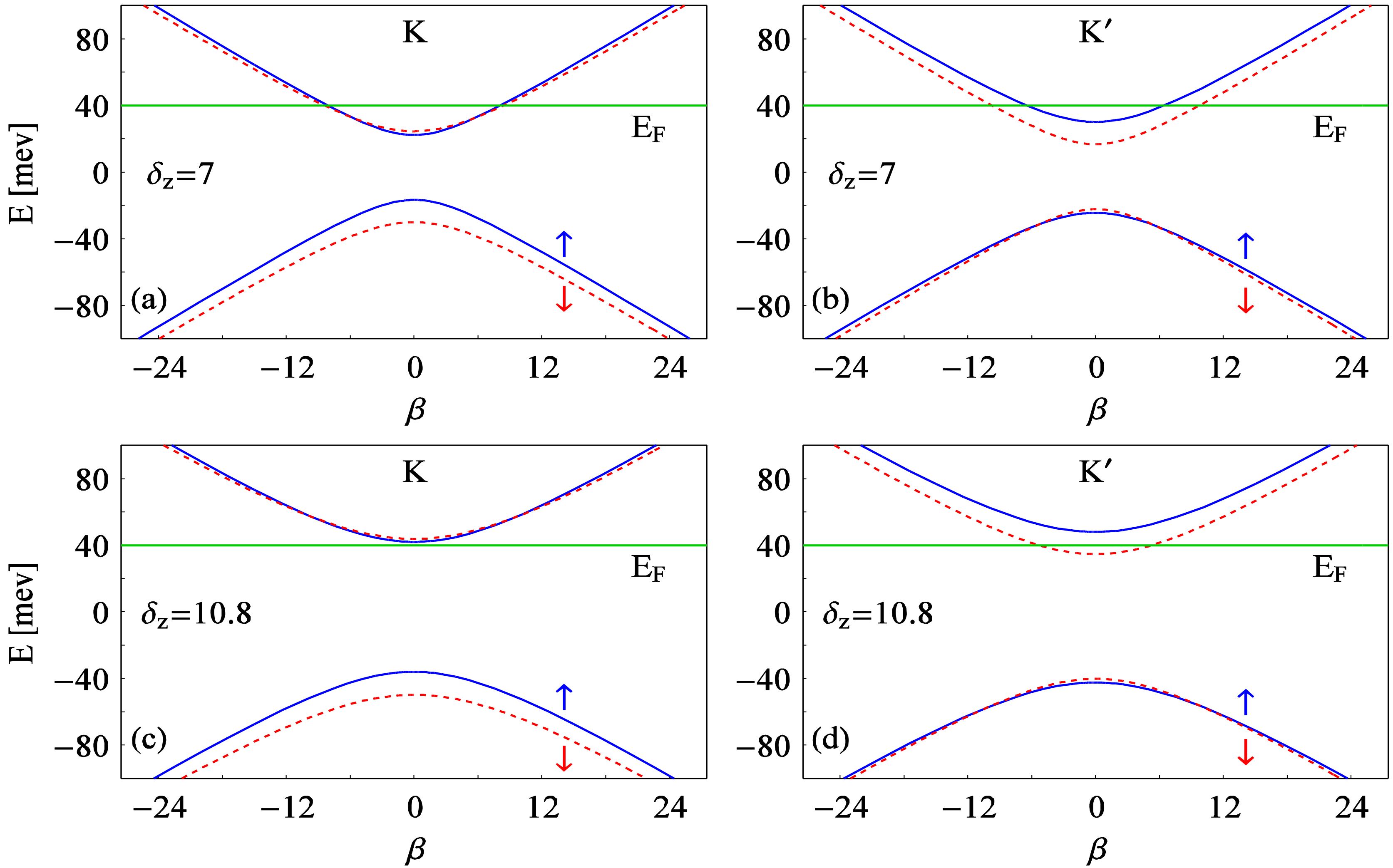
It cannot be made imaginary

For $\Delta_z > \Delta_z^c$ the Fermi level lies in the gap

The junction acts as an electric switch

Band structure $M \neq 0$

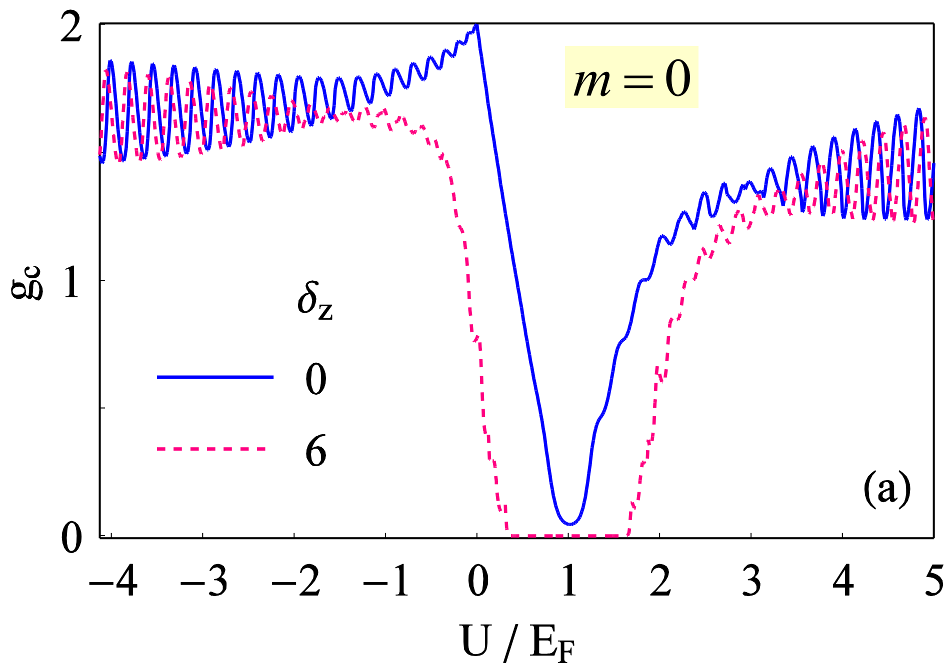
$\delta_z = \Delta_z / \lambda_{so}$ $\beta = \hbar \upsilon_F k / \lambda_{so}$

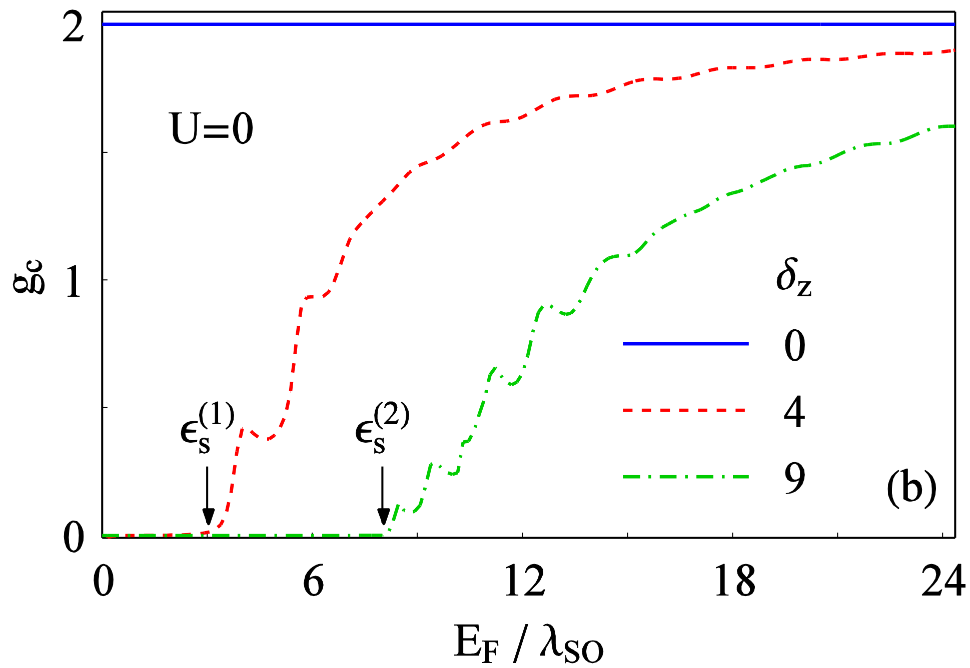


Current is entirely carried by **spin-down electrons** at the K' ($g_\downarrow$ oscillatory)

Only **evanescent modes** contribute to $g_\uparrow$ (monotonically decreasing behavior)

Conductance and transport gap





Near the DP k'_F is imaginary

$$\varepsilon_s^{(1,2)} = E_F^{c(1,2)} / \lambda_{so}$$

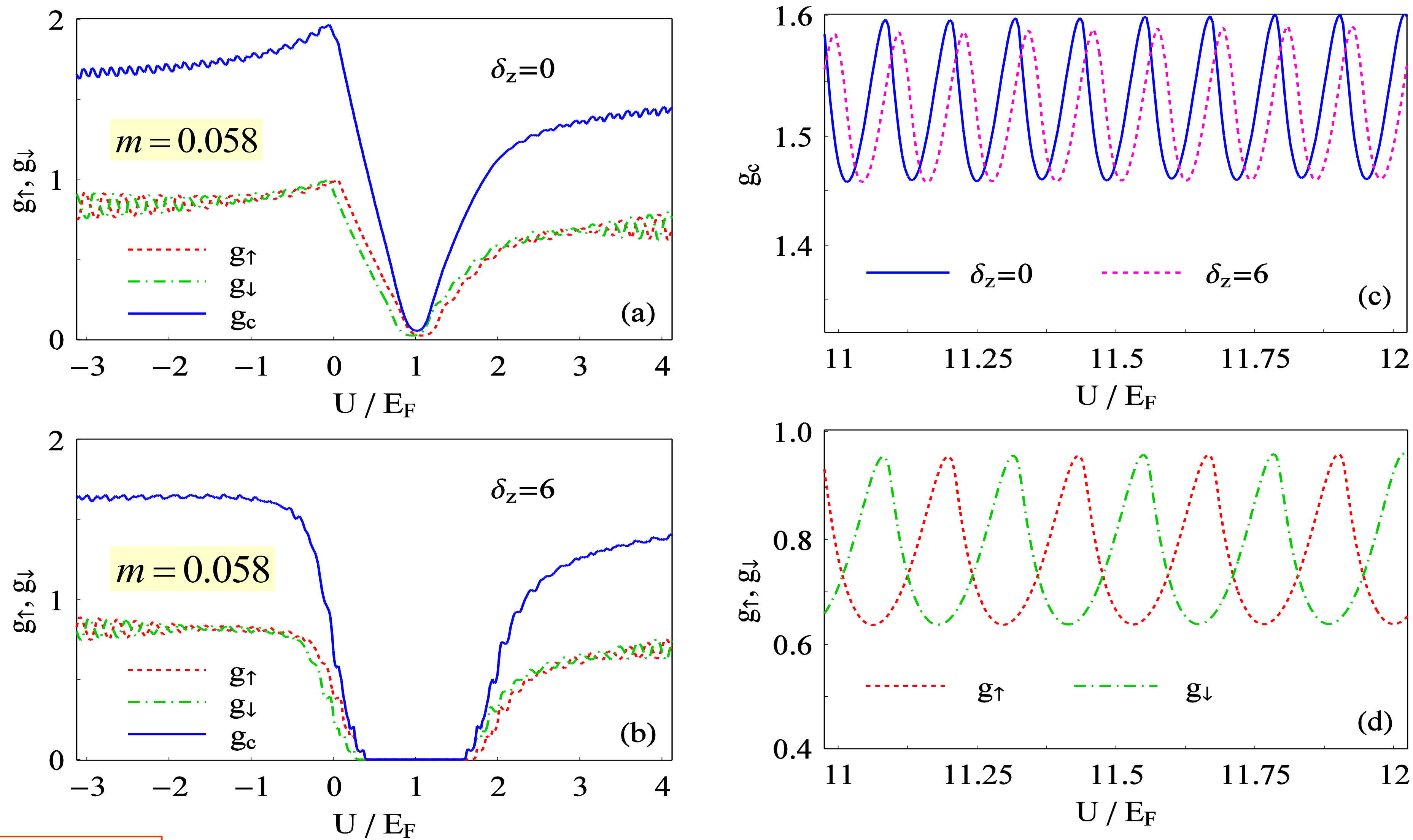
Transport gap when $E_F < E_F^c$

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

$$E_F^c = \Delta_z - \lambda_{so}$$

We aim now to explore possible spin and valley polarizations in FM silicene

Spin-resolved and charge conductances



$m = M / E_F$

Relative sift of $g_\uparrow$ and $g_\downarrow$ in the presence of M

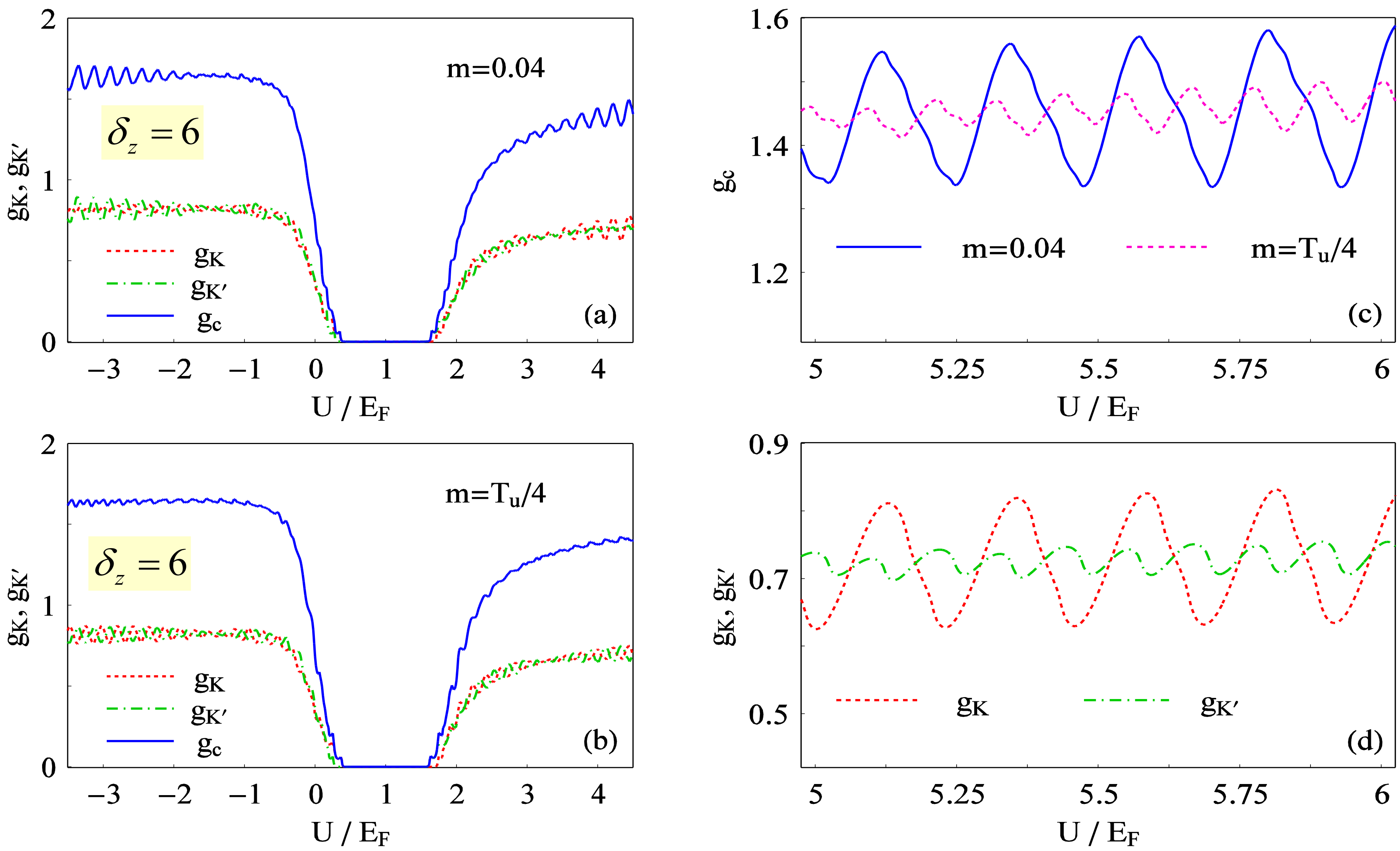
Transport gaps for both

g_c is periodic function of U/E_F

$T_u = \pi\hbar\upsilon_F / E_F d\delta_\lambda$ =0.235

for $|U/E_F| >> 1$

Valley-resolved and charge conductances

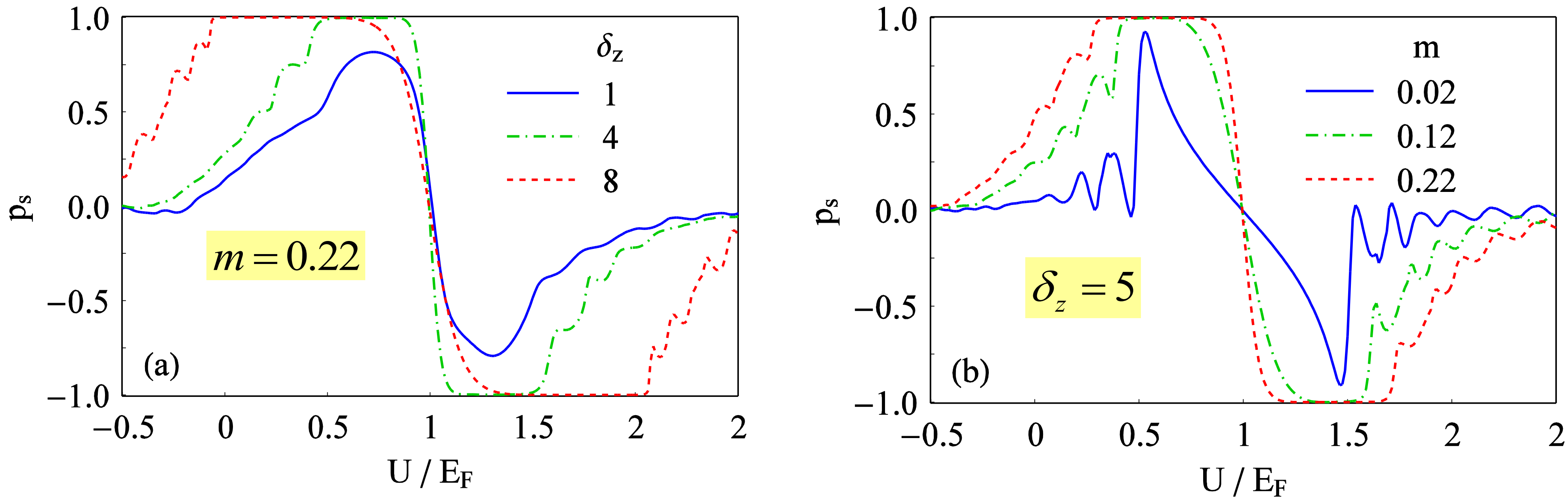


$$g_{K(K')} = \frac{g_{K(K')\uparrow} + g_{K(K')\downarrow}}{2}$$

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



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

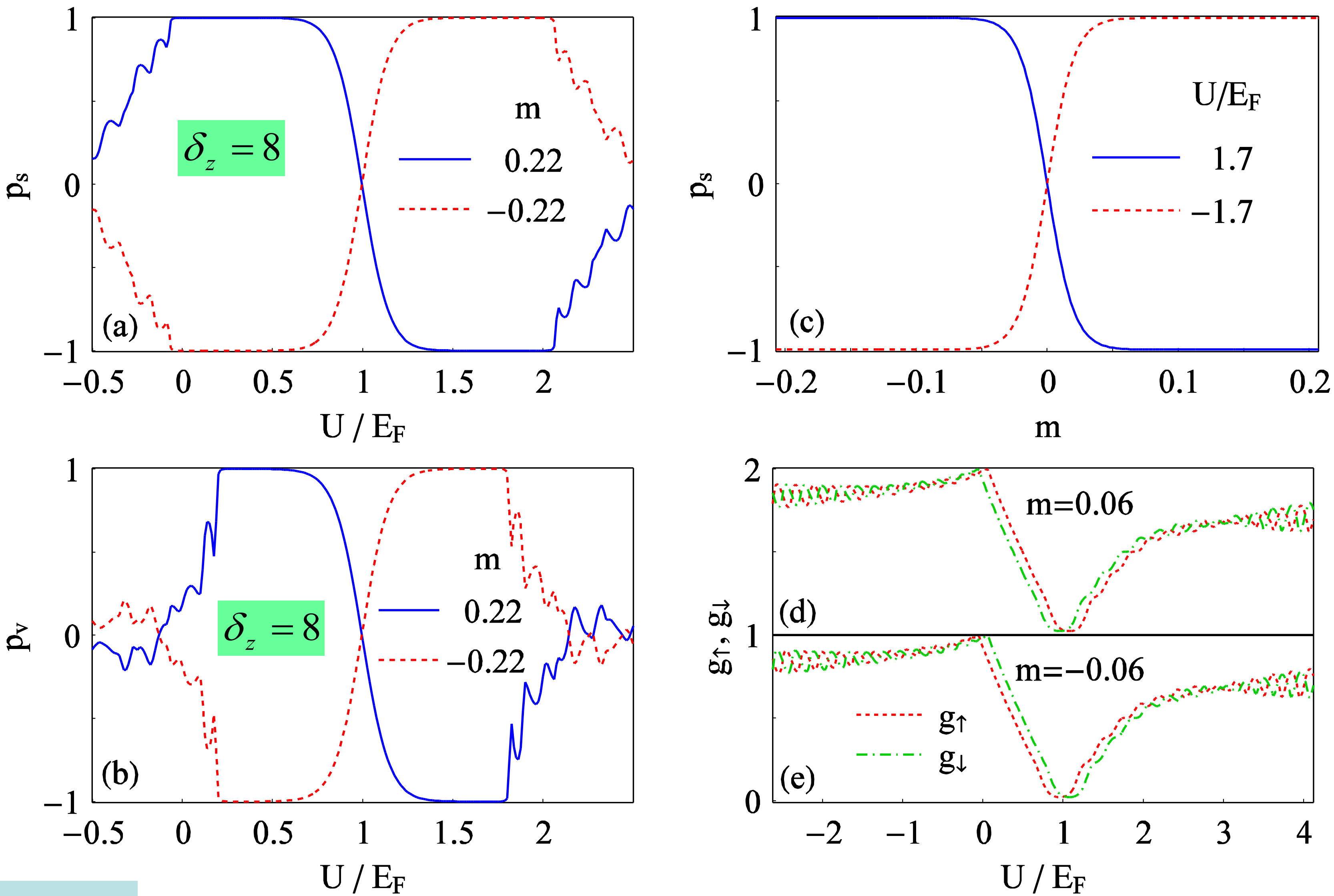
The range of $p_s \approx 1$ increases with δ_z or m

For large δ_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



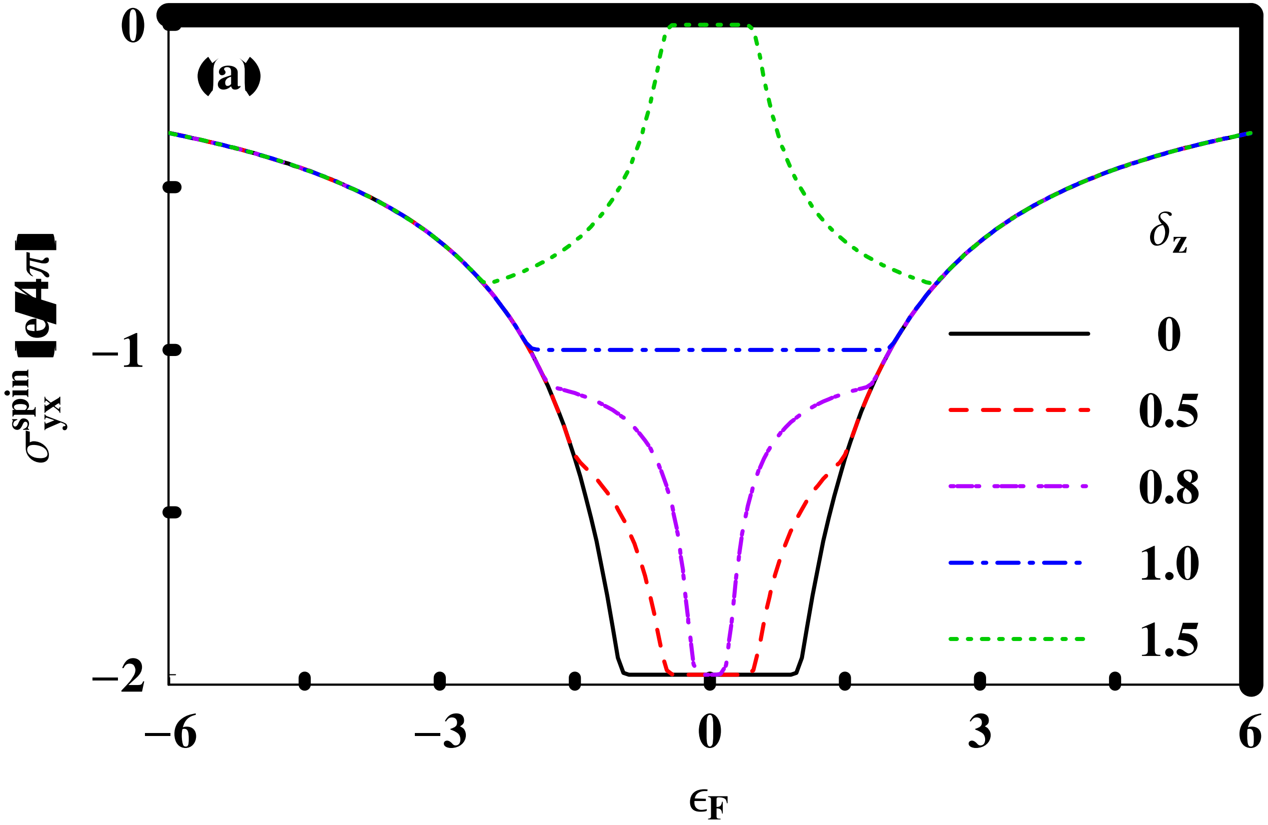
$$p_s = \frac{g_\uparrow - g_\downarrow}{g_\uparrow + g_\downarrow}$$

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

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)