Local currents in a two-dimensional topological insulator

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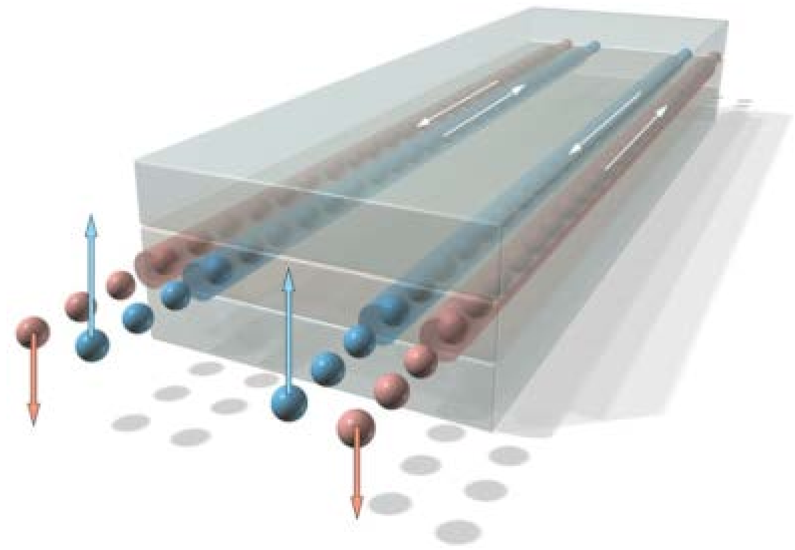
Two-dimensional topological insulator



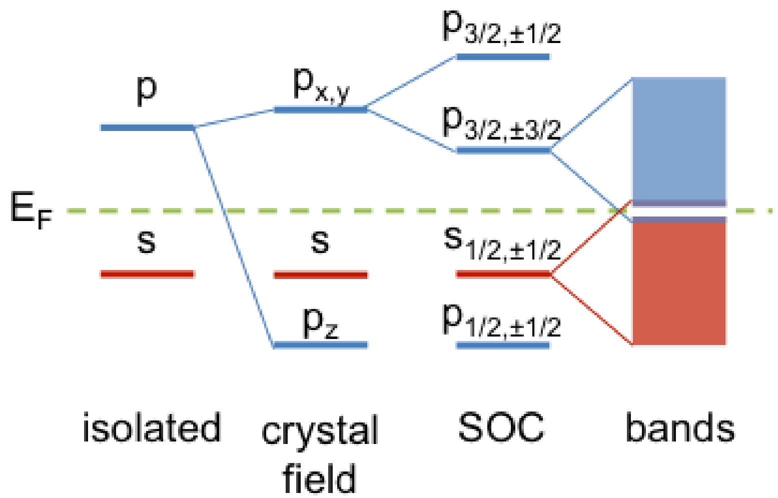
Predicted (Bernevig, Hughes, and Zhang, 2006) and observed (König et al., 2007) in CdTe/HgTe/CdTe quantum well structures

- System exhibiting a quantum spin-Hall effect
- 2D bulk insulator with topologically protected edge states
- Spin is locked to the wave vector of the electron
- Conductance of the edge state is insensitive to disorder which does not break time reversal symmetry

Bernevig-Hughes-Zhang (BHZ) model

BHZ, Science **314**,1757(2006)
Fu and Kane, PRB 76, 045302 (2007)

“Inverted” band structure



$$\varepsilon_s - \varepsilon_p > 4(t_{ss} + t_{pp})$$ - band insulator

$$\varepsilon_s - \varepsilon_p < 4(t_{ss} + t_{pp})$$ - topological insulator

Square lattice with four basis states α on each site i:

$$|s,\uparrow\rangle \quad |s,\downarrow\rangle \quad |p_x + ip_y,\uparrow\rangle \quad |p_x - ip_y,\downarrow\rangle$$

Hamiltonian:

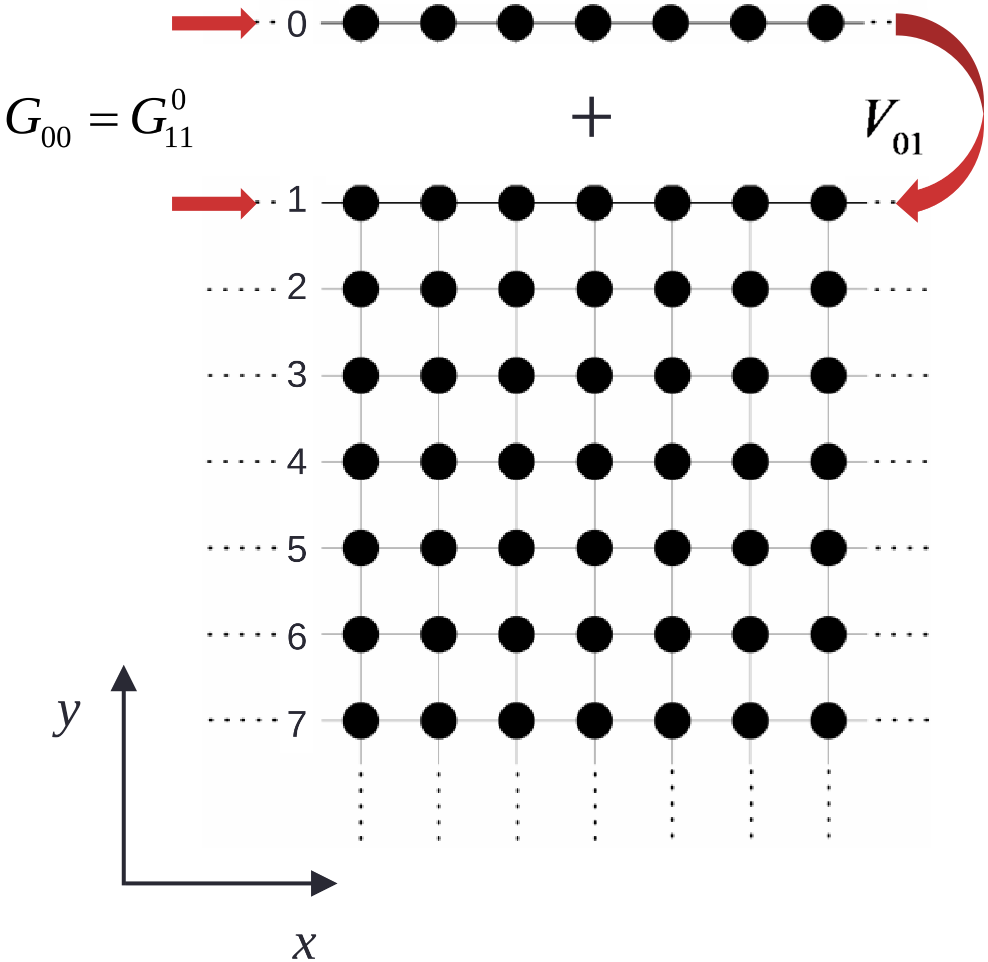
$$H = \sum_{i,\sigma,\alpha} \varepsilon_\alpha c^\dagger_{i\alpha\sigma} c_{i\alpha\sigma} - \sum_{i,\sigma,\alpha} t_{a\sigma,\alpha\beta} c^\dagger_{i+a\alpha\sigma} c_{i\beta\sigma}$$

$$t_{a\sigma} = \begin{pmatrix} t_{ss} & t_{sp} e^{i\sigma\theta_a} \\ t_{sp} e^{-i\sigma\theta_a} & -t_{pp} \end{pmatrix}$$

θ_a - angle of bond a with x axis

Tight-binding Green's function technique

Semi-infinite square lattice



Dyson equation:

$$G = G^0 + G^0 V G$$

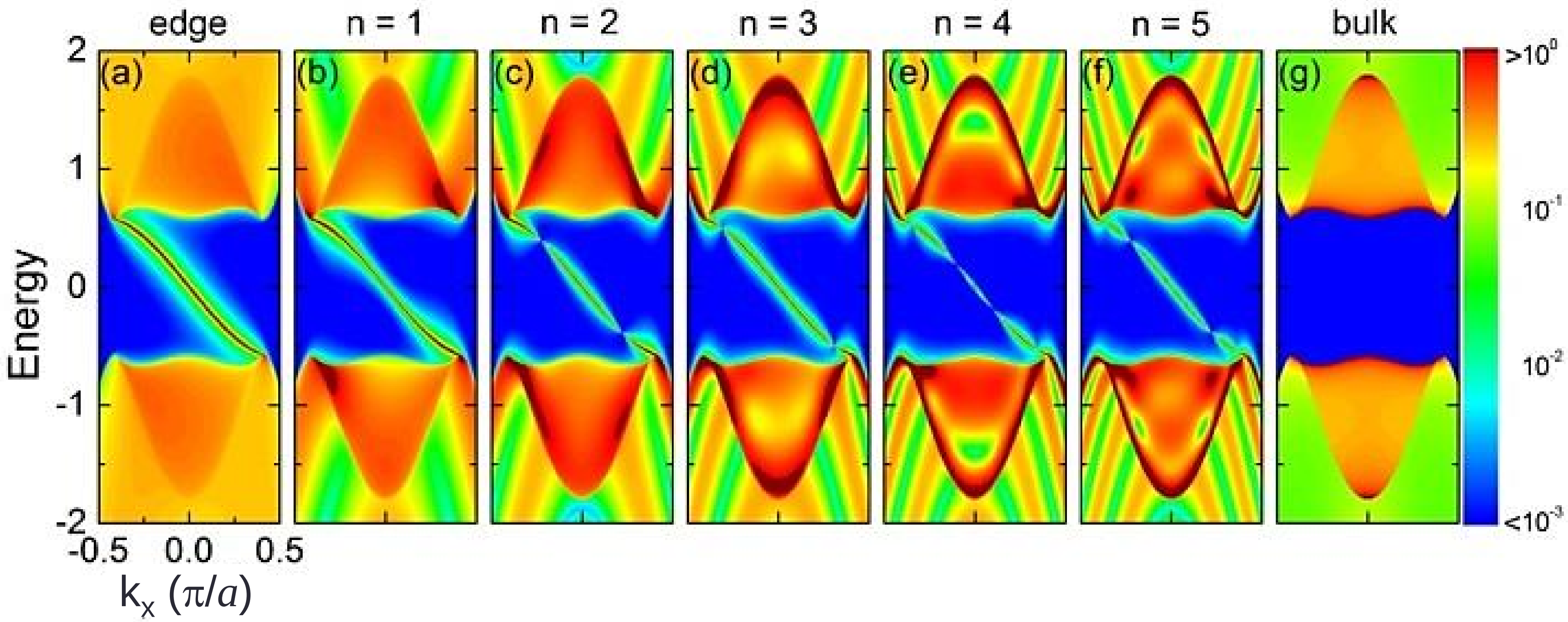
Layer-dependent spectral density:

$$A_n(E,k_x) = -\mathrm{Im}\left[Tr G_{nn}(E,k_x)\right]$$

Layer-dependent DOS:

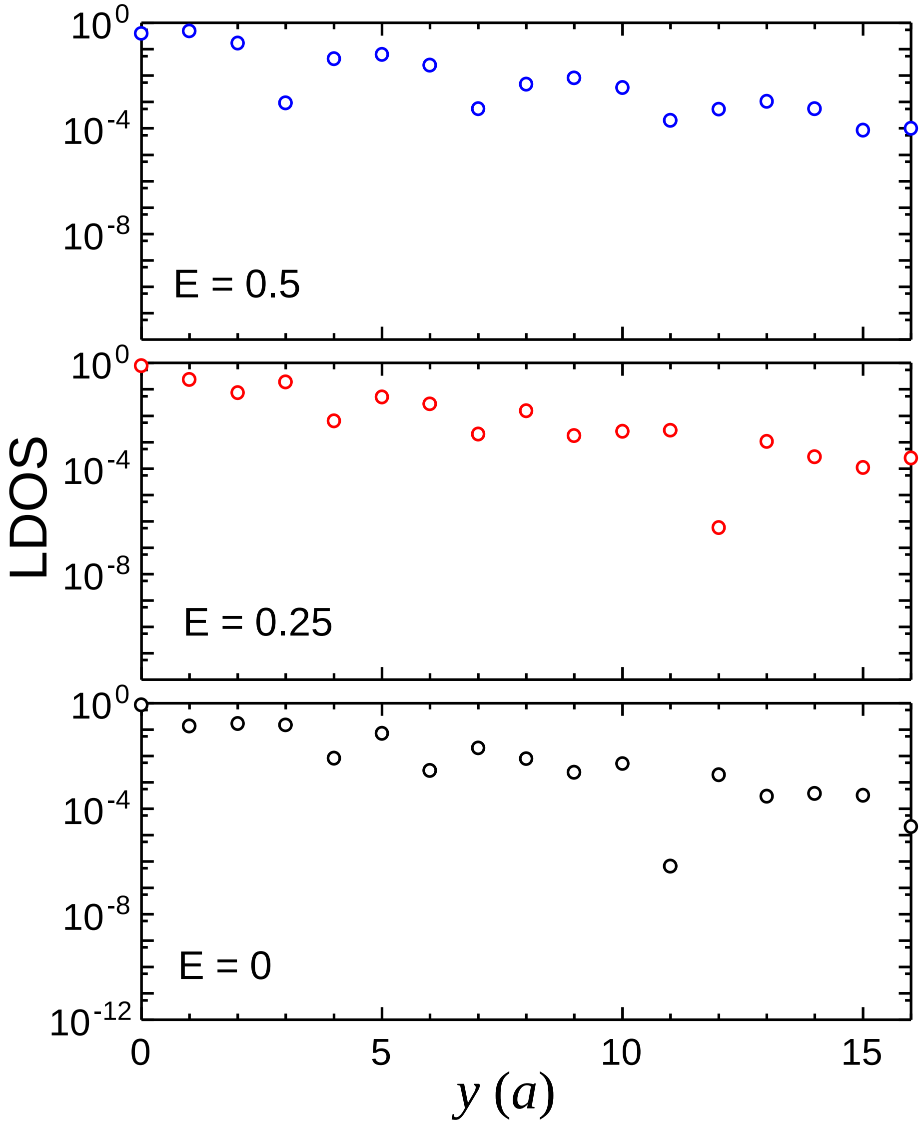
$$\rho_n(E) = -\frac{1}{\pi}\mathrm{Im}\left[Tr G_{nn}(E)\right]$$

Layer-dependent spectral density



- Energy dependent oscillatory decay of the edge state into the bulk

Oscillatory decay of DOS

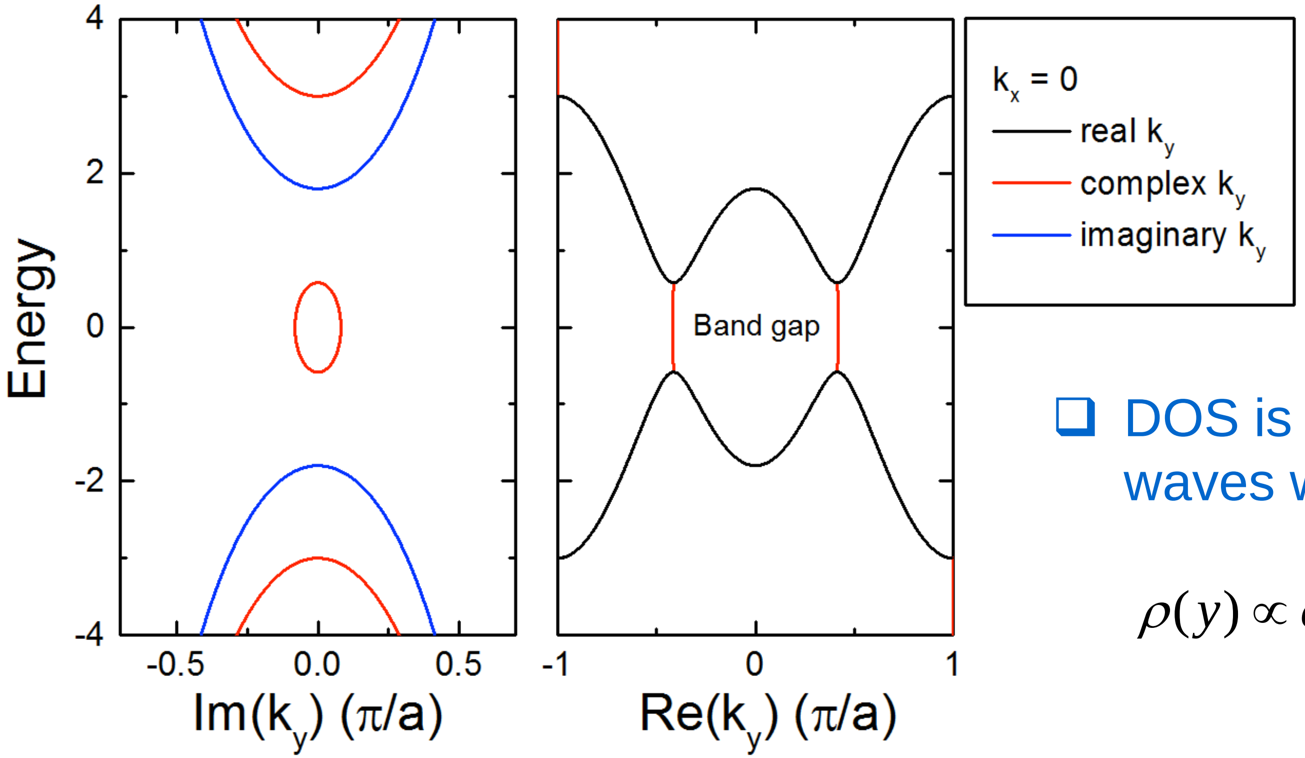


- Oscillatory decay of the edge state into the bulk

Complex band structure

For a given energy, there are three types of solutions:

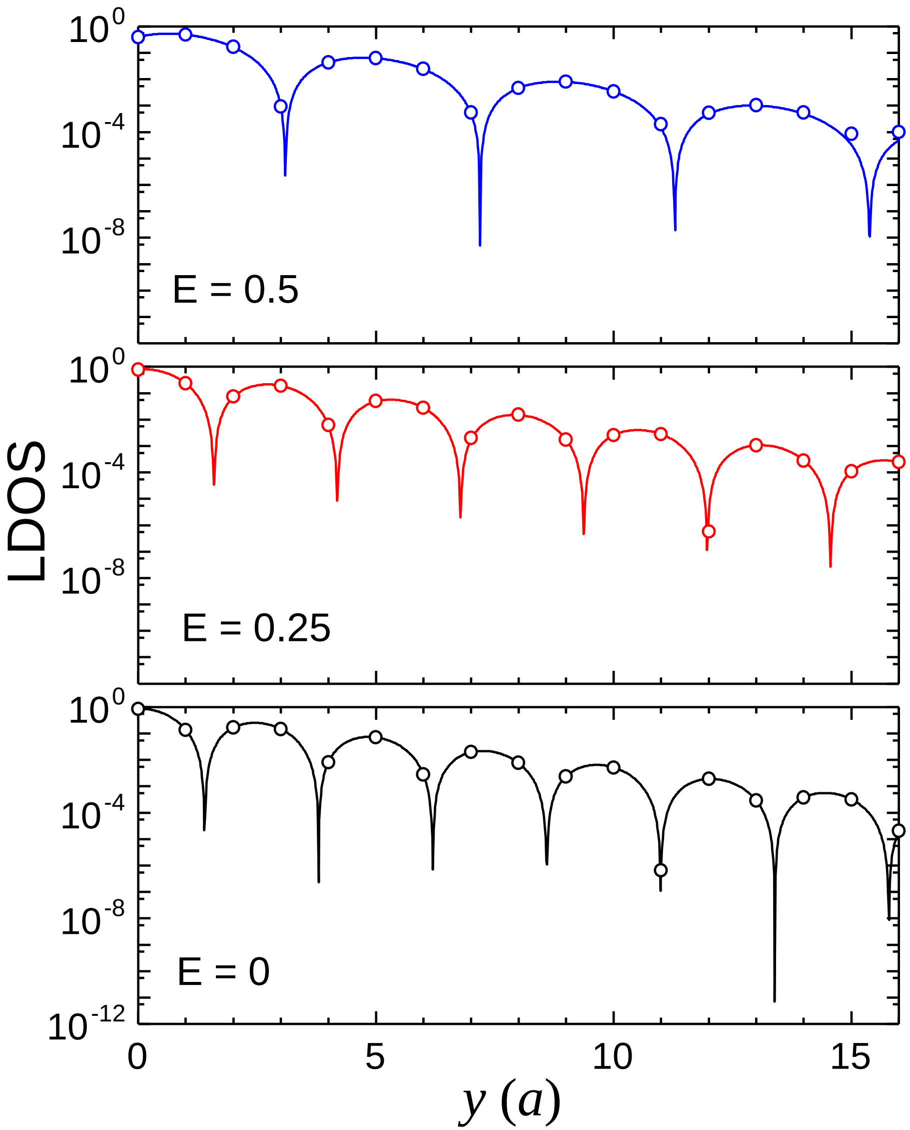
- Bloch state : $\varphi \sim e^{ik_y y}$ - oscillation
- Evanescent state: $\varphi \sim e^{-\kappa y}$ - decay
- Complex solution: $\varphi \sim e^{ik_y y} e^{-\kappa y}$ - oscillation and decay



- DOS is superposition of two waves with opposite Re(k_y):

$$\rho(y) \propto e^{-2\kappa y} \cos^2\left(k_y y + \phi\right)$$

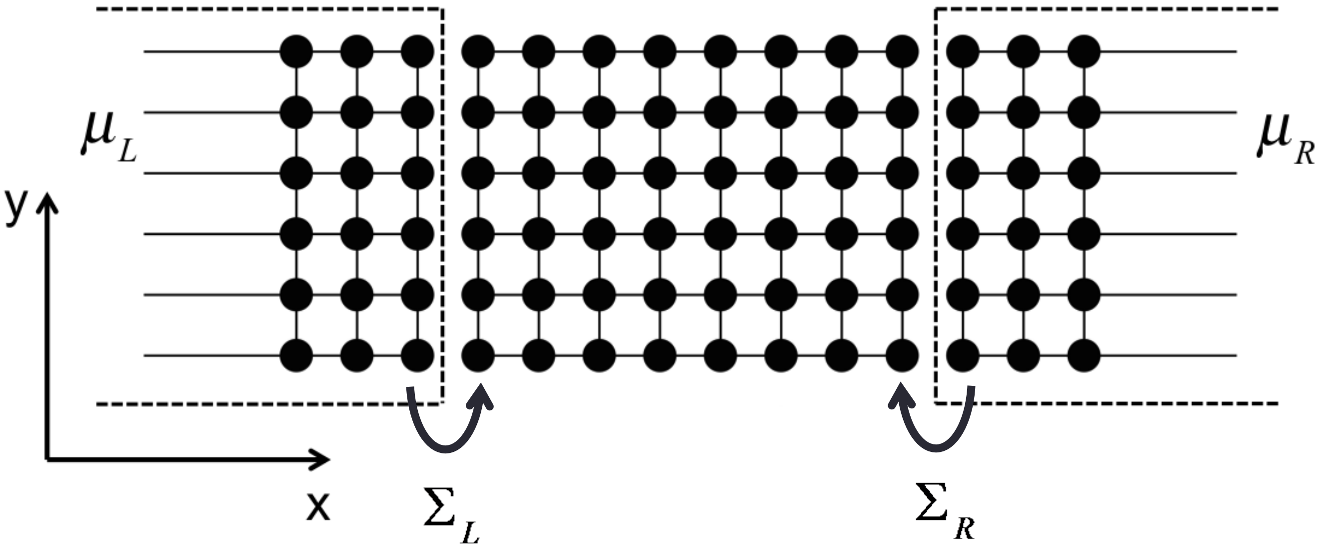
Oscillatory decay of DOS



Layer-dependent DOS using parameters extracted from the complex band structure

$$\rho(y) \propto e^{-2\kappa y} \cos^2\left(k_y y + \phi\right)$$

Electronic transport: model and methods



- Finite width strip within the BHZ tight-binding model
- Green's function formalism

$$G(E) = [E - H - \Sigma_L - \Sigma_R]^{-1}$$

- Landauer-Büttiker approach

Local conductance

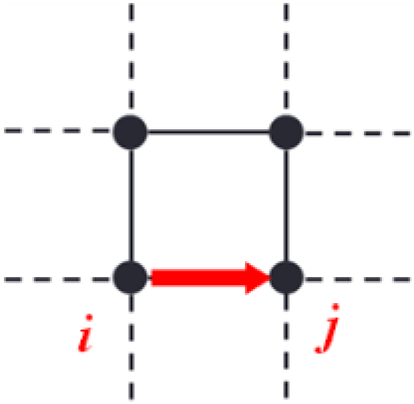
Local current: $I_{ij} = Tr(\rho J_{ij})$

where

$$J_{ij} = \frac{e}{ih}\left[H_{ij} |i\rangle\langle j| - H_{ji} |j\rangle\langle i| \right]$$

$$\rho = \int \left[f_L(E) A_L(E) + f_R(E) A_R(E) \right] dE$$

$$A_{L,R}(E) = iG(E)\left[\Sigma_{L,R}(E) - \Sigma^{\dagger}_{L,R}(E) \right] G^{\dagger}(E)$$



Within linear response

$$\rho = \rho_0 + eV \int \left(-\frac{\partial f_0}{\partial E} \right) A_L(E) dE$$

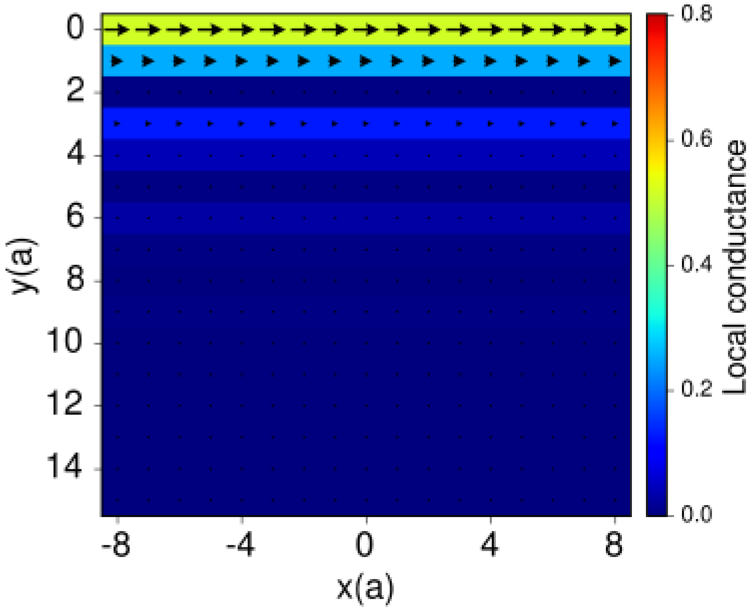
Local conductance (per spin):

$$\Gamma_{ij} = \frac{I_{ij}}{V} = \frac{e^2}{h} \operatorname{Im} Tr\left[A_{Lij}(E_F) H_{ij} - A_{Lji}(E_F) H_{ji} \right]$$

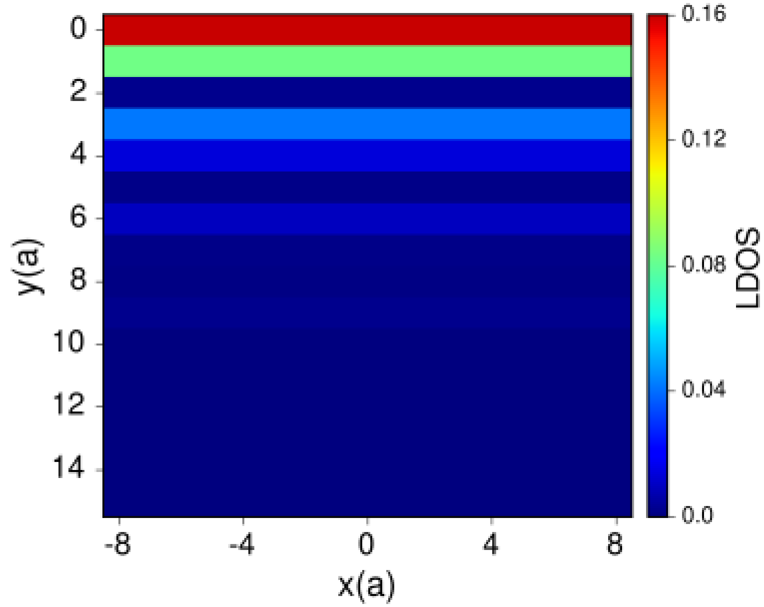
Total conductance (per spin): $\Gamma = \frac{e^2}{h} T = Tr\left[(\Sigma_L - \Sigma_L^{\dagger}) G (\Sigma_R^{\dagger} - \Sigma_R) G^{\dagger} \right]$

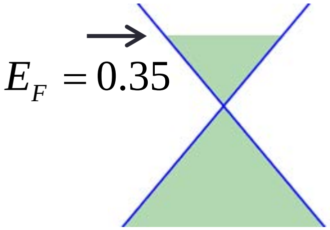
Local conductance for an isolated edge

Local conductance



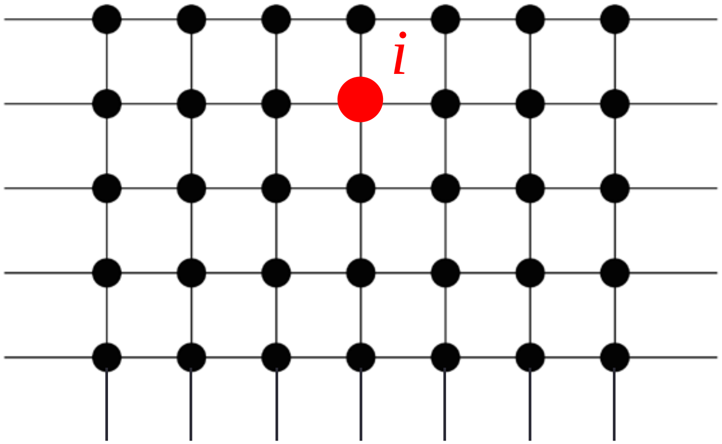
LDOS





- Oscillation in the local conductance
- Correlation between local conductance and local density of states
- Explained by the complex band structure
- T = 1, as expected

Effect of impurity

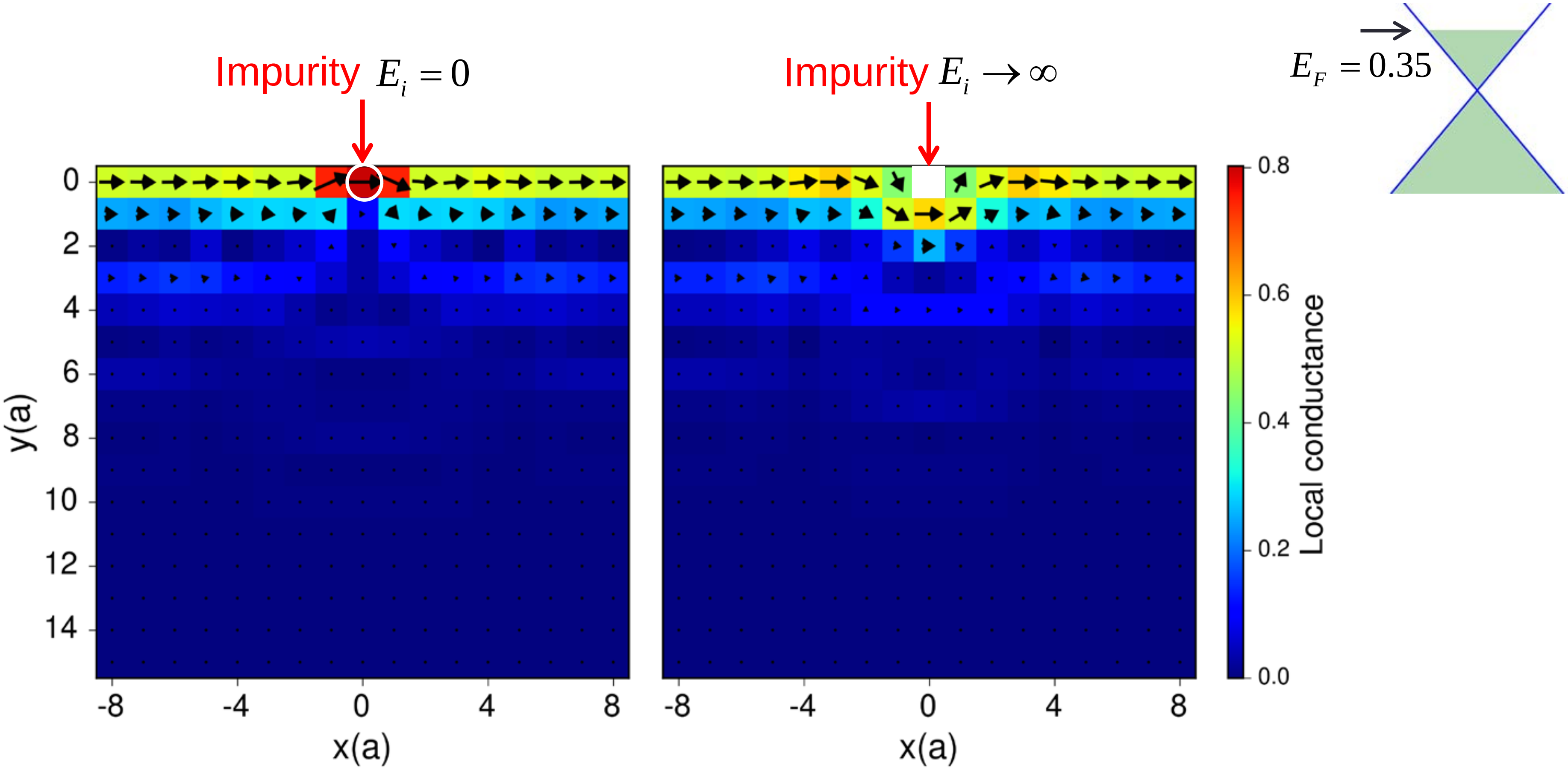


Perturbation due to impurity: $V_{imp} = \begin{pmatrix} \Delta\varepsilon_s & 0 \\ 0 & \Delta\varepsilon_p \end{pmatrix}$

Real space Green's function:

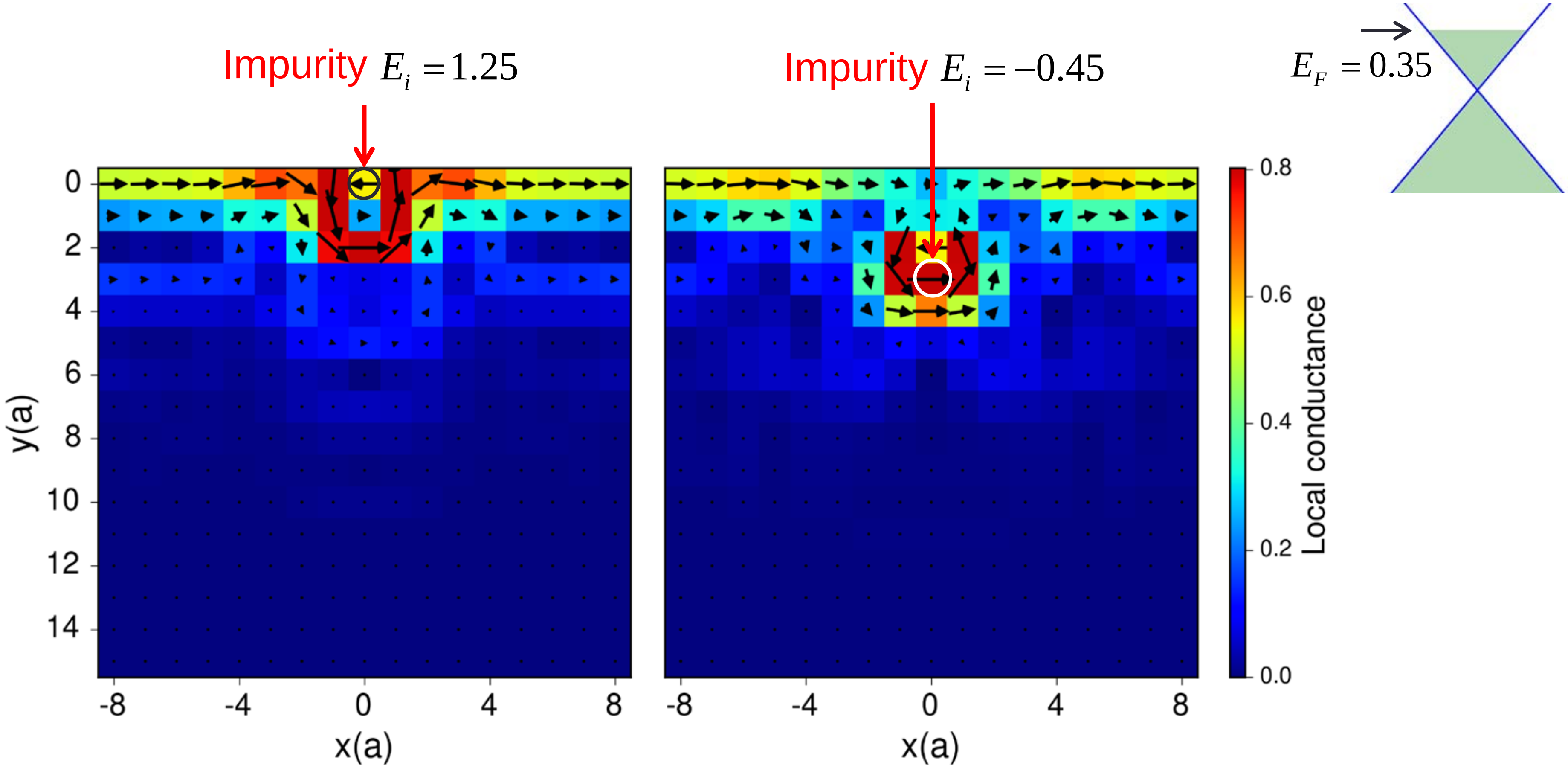
$$G_{mn} = G^0_{mn} + G^0_{mi} V_{ii} \left(1 - G^0_{ii} V_{ii}\right)^{-1} G^0_{in}$$

Effect of impurity



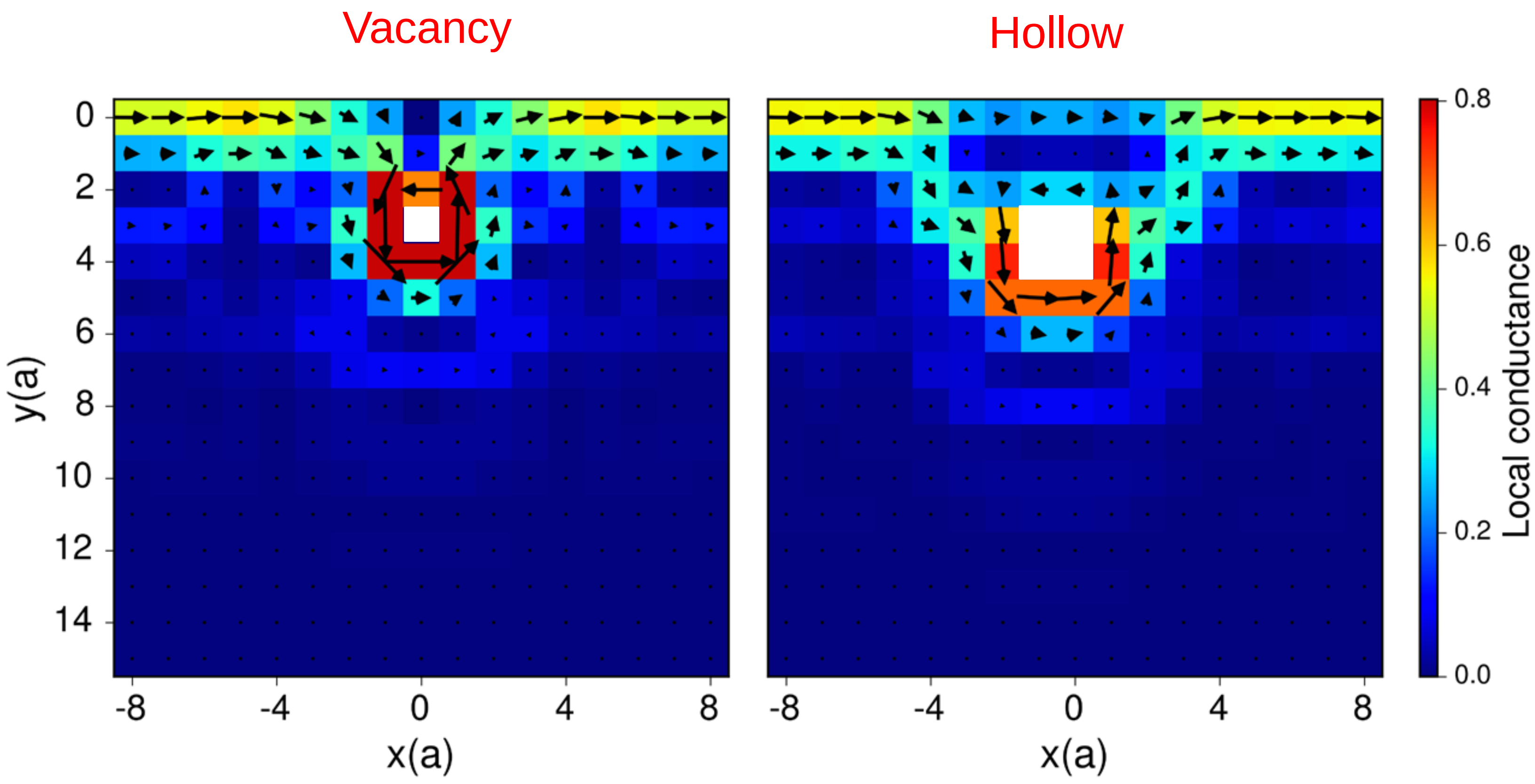
- ❑ Strong effect on local current distribution
- ❑ No back-scattering: T = 1, as expected

Effect of impurity



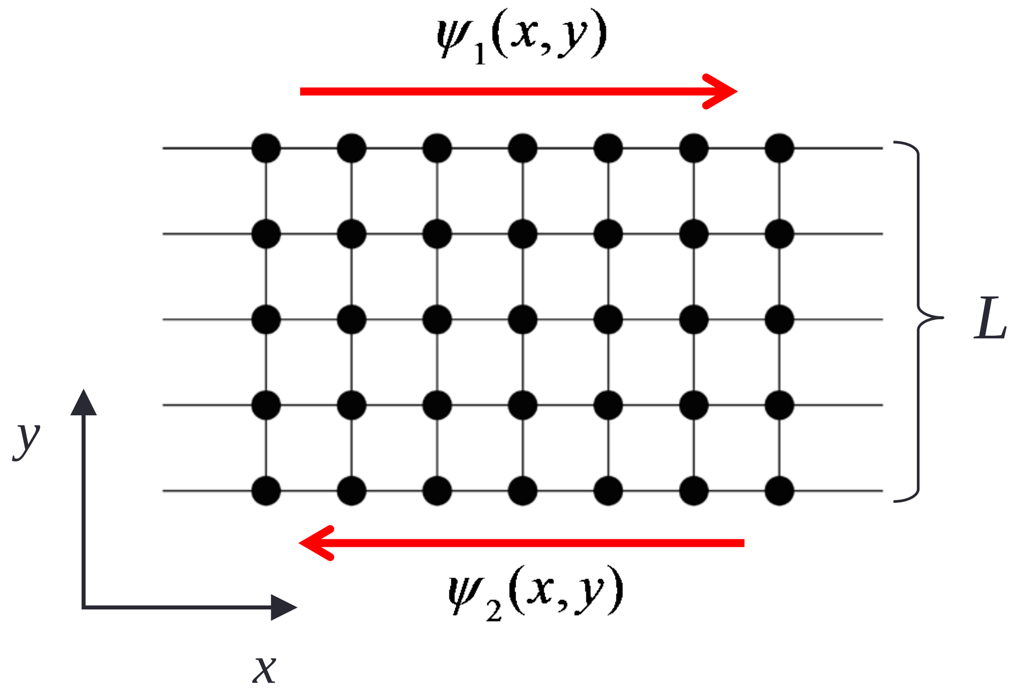
- Intricate current distributions
- Current vortex due to impurity

Effect of vacancy



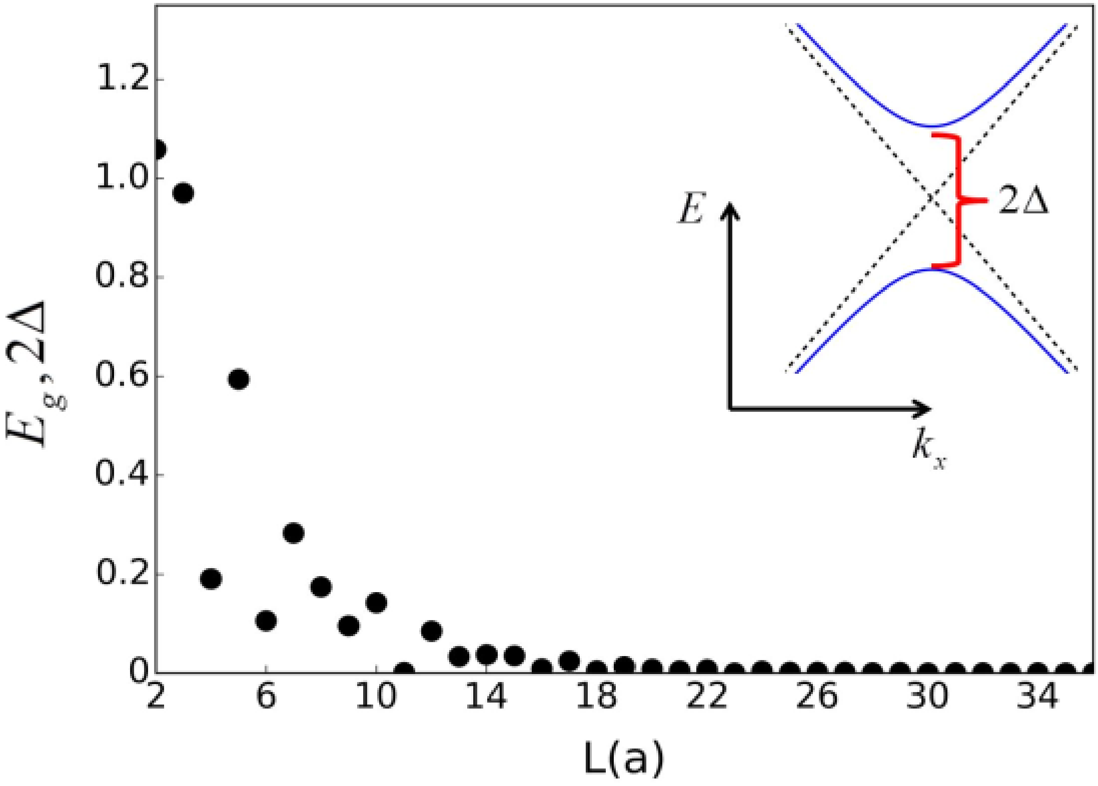
- Current vortex due to internal edge
- Chirality is determined by propagating mode spin state
- Counterclockwise current

Narrow width strip



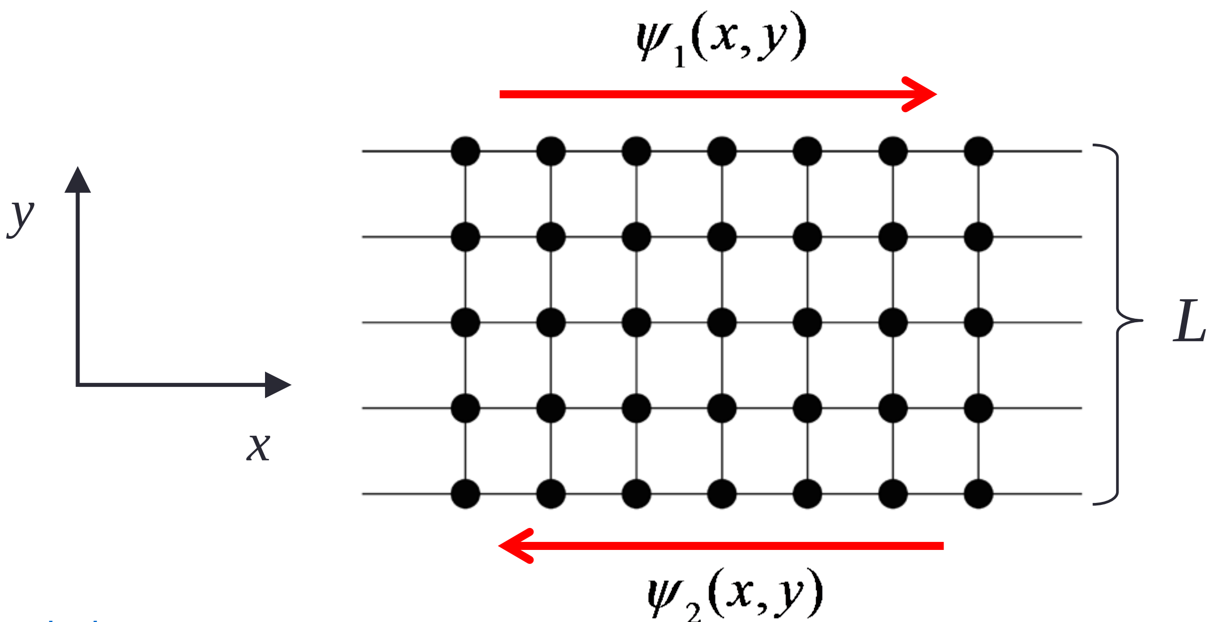
- For a given spin, two propagating states on the two edges
- Coupling between the edge states
- Backscattering due to impurities

Oscillatory band gap



- Energy gap due to coupling between the edge states
- Oscillatory behavior as a function of strip width

Oscillatory band gap



Edge states:

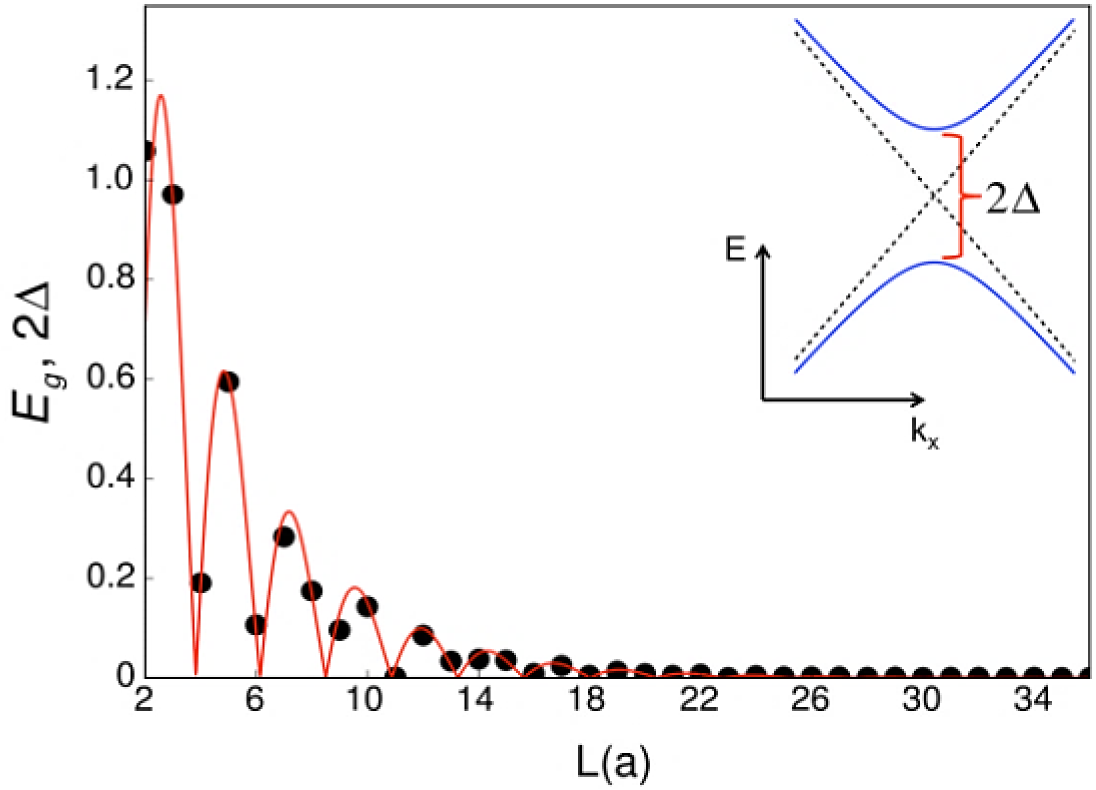
$$\psi_1(x,y) \propto e^{-\kappa y}\left(e^{iky} + re^{-iky}\right)e^{ik_x x}$$

$$\psi_2(x,y) \propto e^{-\kappa(L-y)}\left(e^{ik(L-y)} + re^{-ik(L-y)}\right)e^{-ik_x x}$$

Energy gap:

$$E_g \propto \left|\langle\psi_1|\psi_2\rangle\right| = e^{-\kappa L}\left|\cos(kL) + \frac{\alpha}{L}\sin(kL)\right|, \qquad \alpha = (1+r^2)/4rk$$

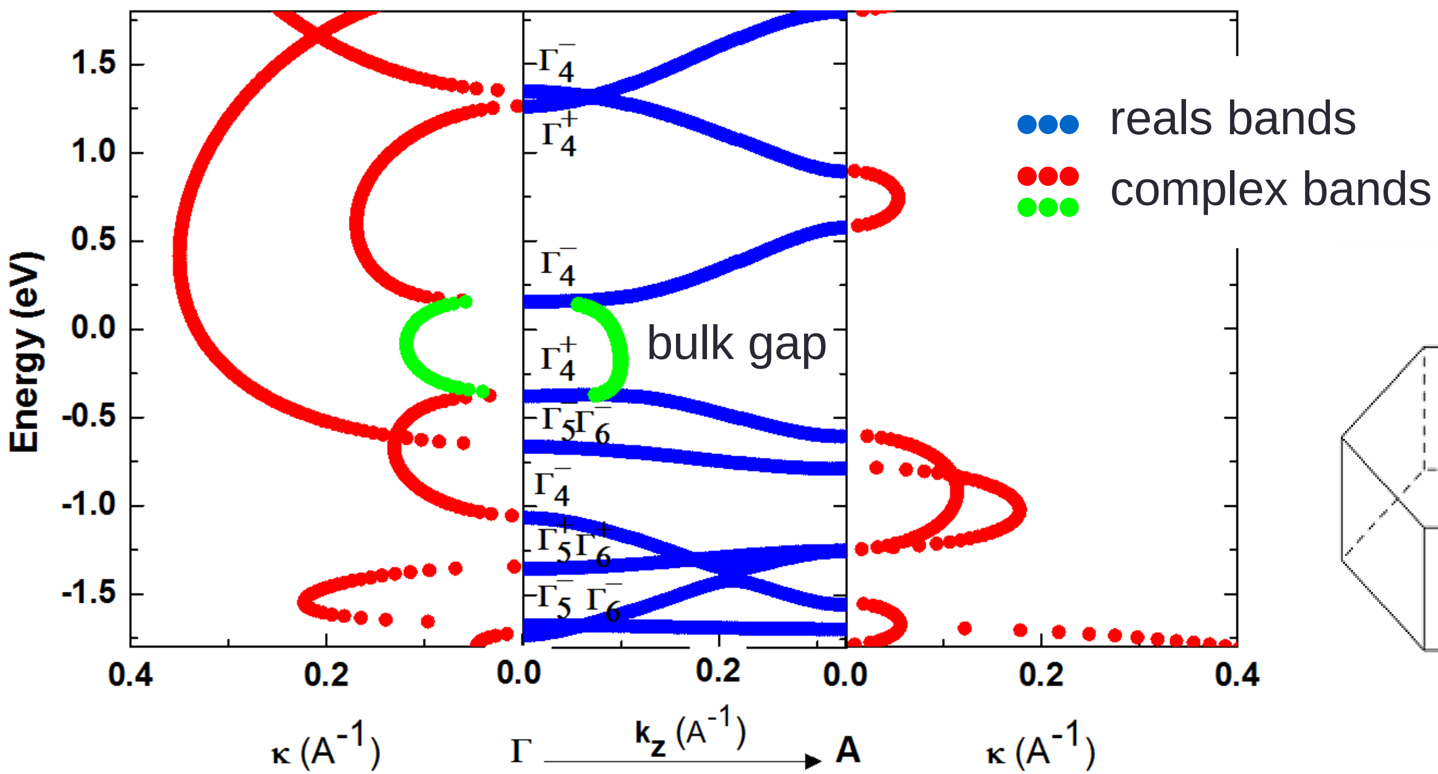
Oscillatory band gap

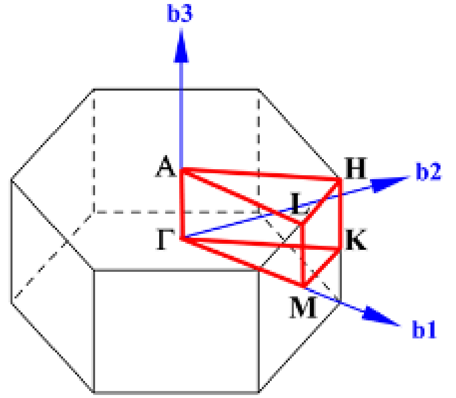


- Excellent agreement

Complex band structure of Bi_2Se_3

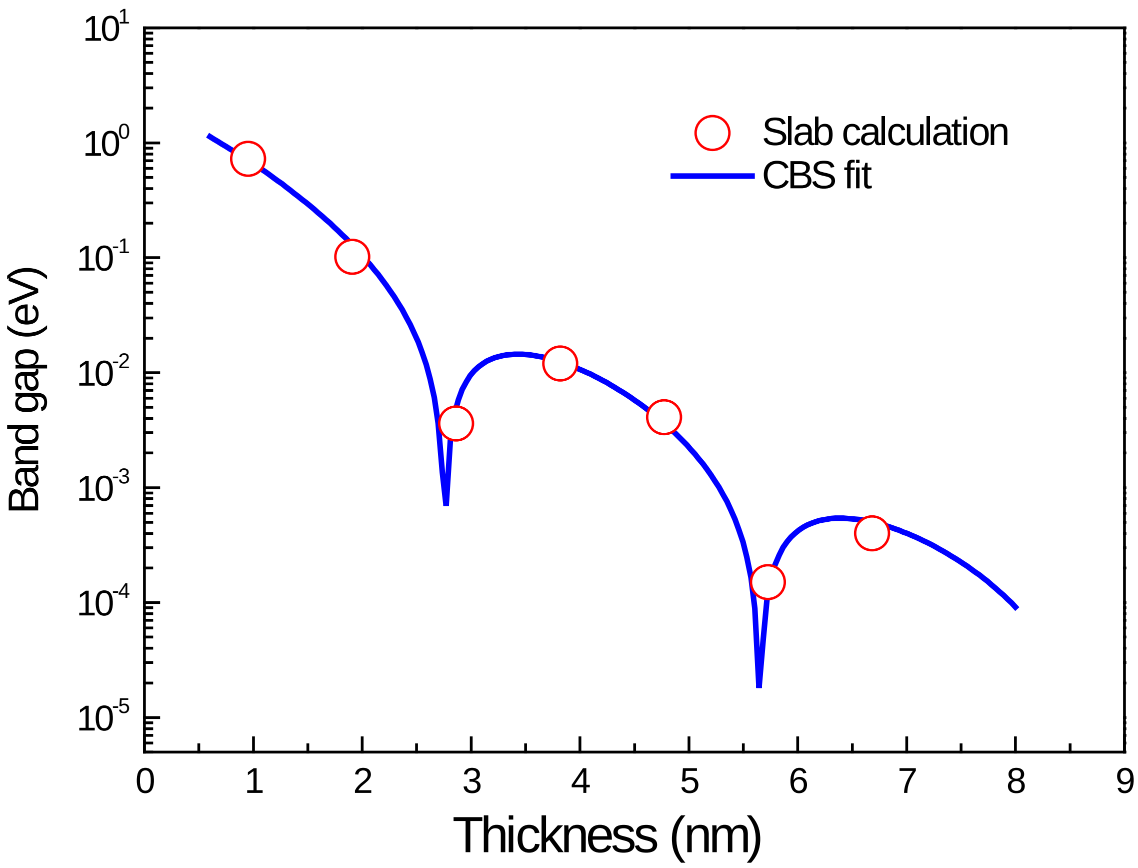
In collaboration with J. Velev (UPR)

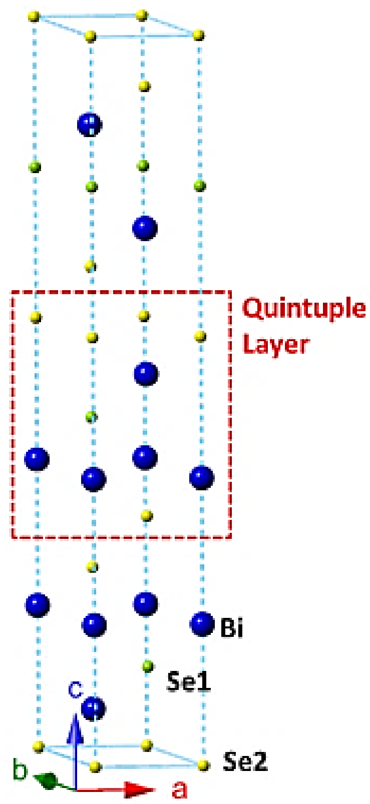




❑ Real component of the wave vector in the bulk gap region

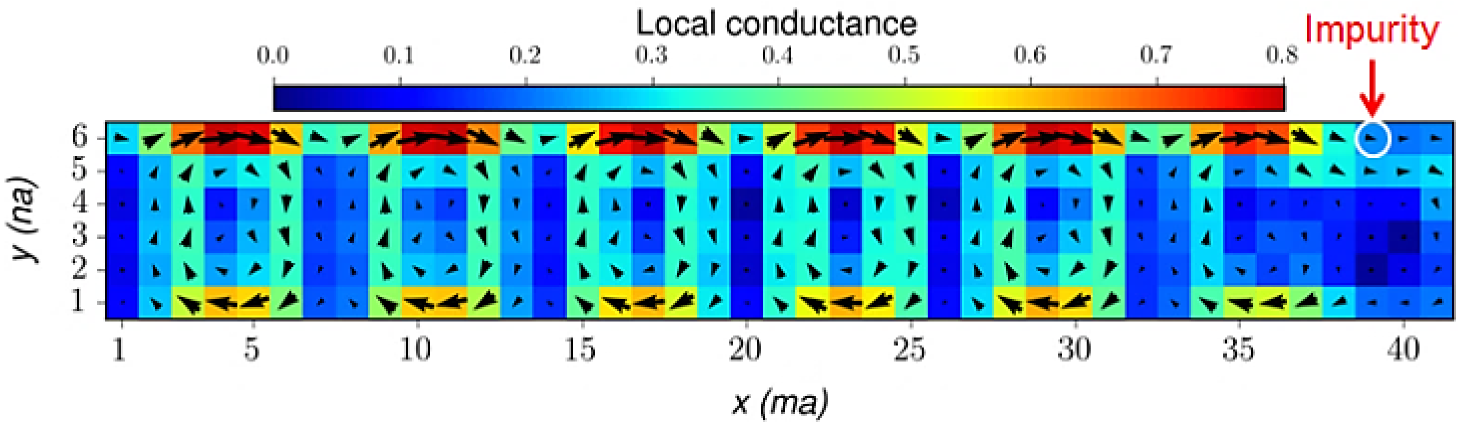
Oscillatory band gap in Bi_2Se_3

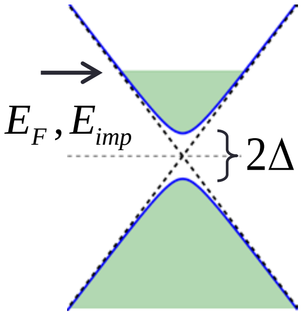




❑ Nearly perfect agreement with the complex band structure parameters

Friedel oscillations: density of states





- No Friedel oscillations for an isolated edge
- For a finite strip, LDOS oscillates away from the impurity with no decay
- Oscillation period depends on the Fermi energy

Friedel oscillations: model

Model Hamiltonian: $$H(k) = \begin{pmatrix} \hbar v k & \Delta \\ \Delta & -\hbar v k \end{pmatrix}$$

Green's function:

$$G_0(x - x', E) = \frac{-i}{2\hbar^2 v^2 k} e^{ik|x-x'|} \begin{pmatrix} E + \hbar v k \operatorname{sgn}(x - x') & \Delta \\ \Delta & E - \hbar v k \operatorname{sgn}(x - x') \end{pmatrix}$$

Dyson equation within Born approximation:

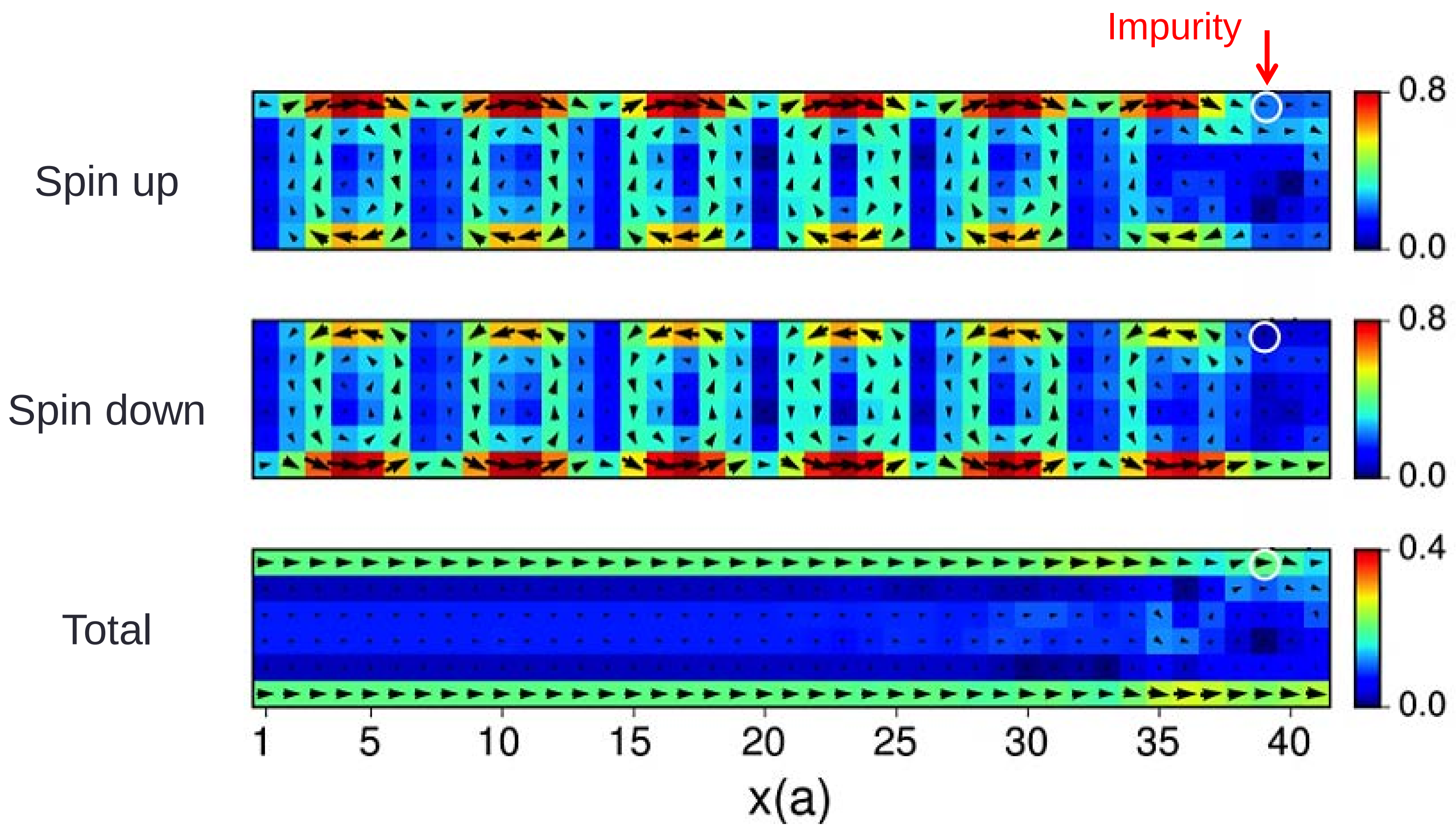
$$G(x, x', E) \approx G_0(x, x', E) + \int_{-\infty}^{\infty} G_0(x - x'', E) V(x'') G_0(x'' - x', E) dx''$$

where $V(x) = \lambda \delta(x)$ is a local perturbation due to impurity

Resulting perturbation in LDOS:

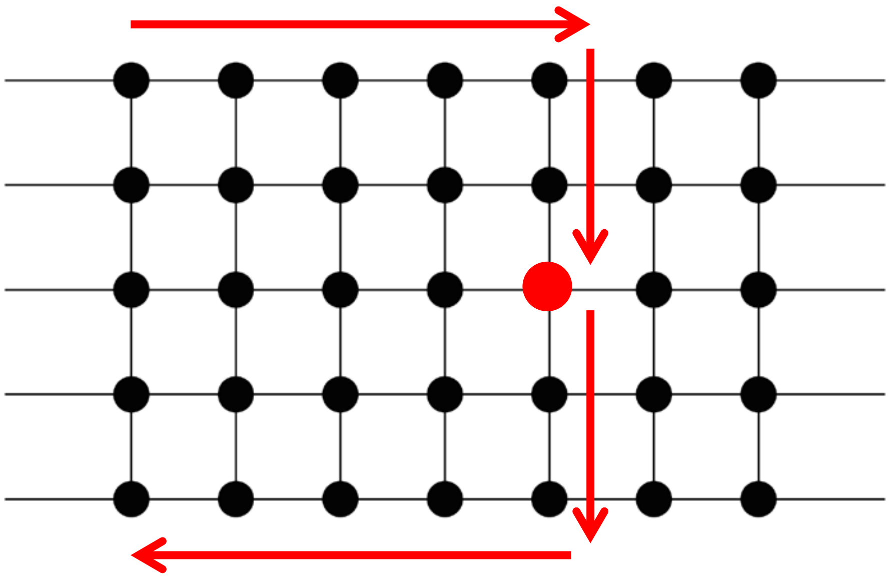
$$\Delta\rho(x) = -\frac{1}{\pi} \operatorname{Im} \operatorname{Tr}[G - G_0] = \frac{\lambda \Delta^2}{\pi \hbar^4 v^4} \frac{\sin(2k_F |x|)}{k_F{}^2}$$

Friedel oscillations: local conductance



- ❑ Periodically repeated vortices in spin-resolved current distribution
- ❑ No Friedel oscillations in net local conductance

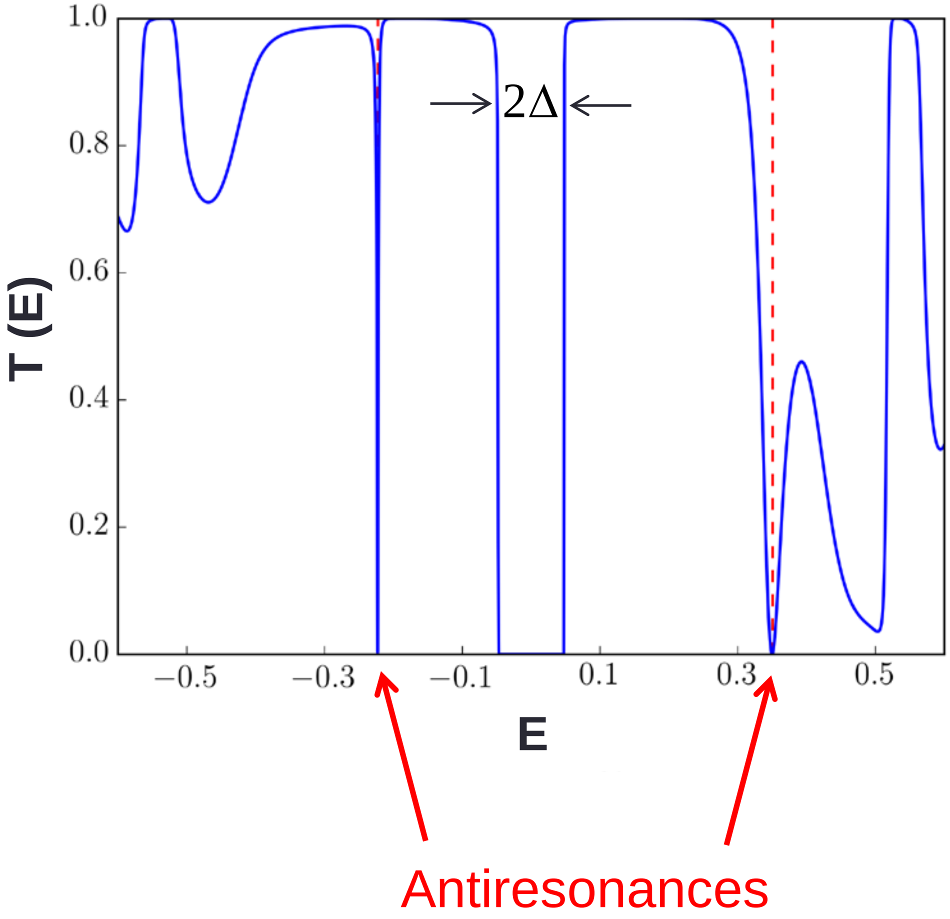
Resonant scattering



- Resonant channel: full back-scattering due to bound state created by impurity

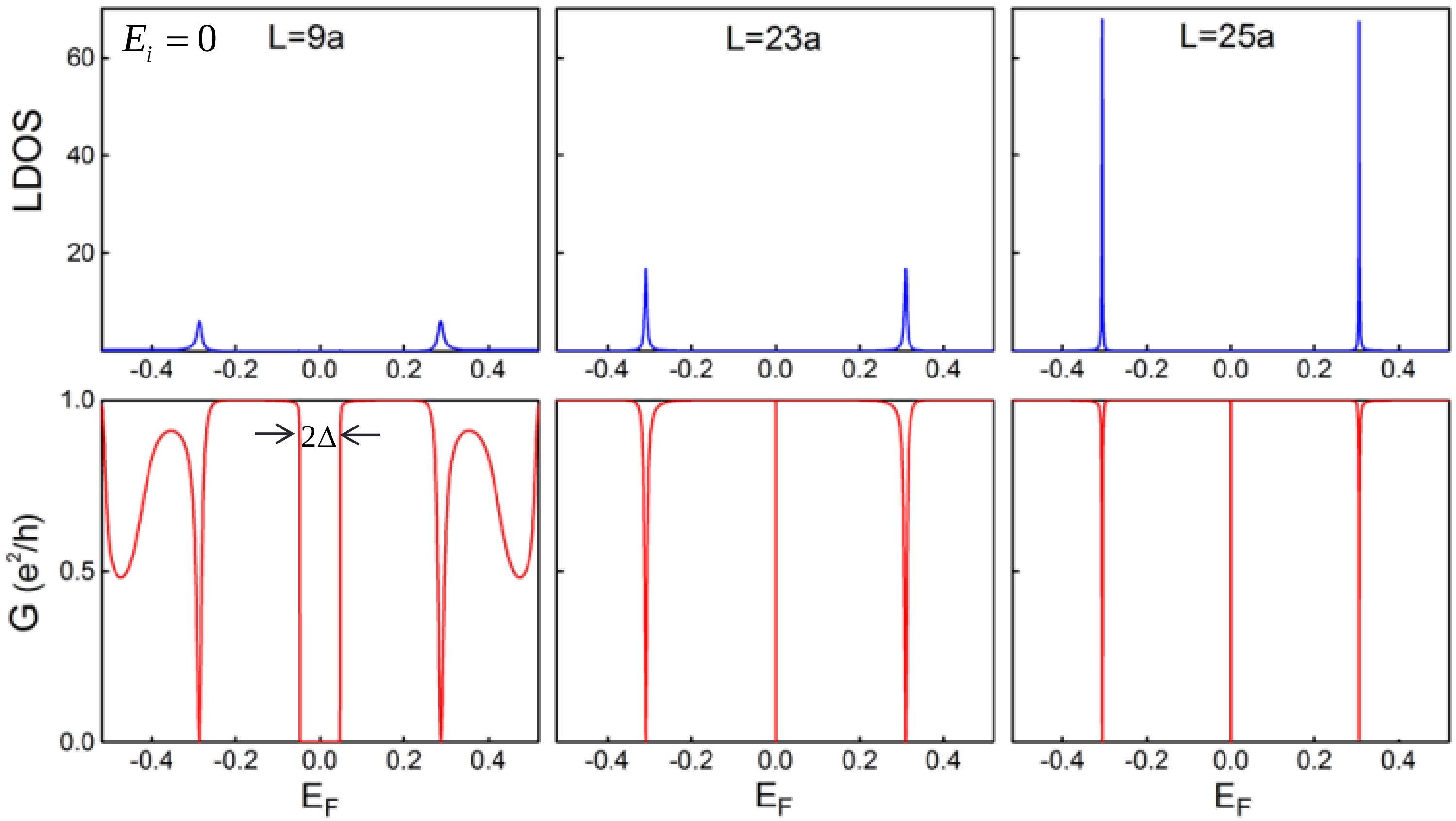
Resonant scattering: antiresonance

Energy dependent transmission



- ❑ Full suppression of net current
- ❑ Destructive interference of the incoming and reflected waves

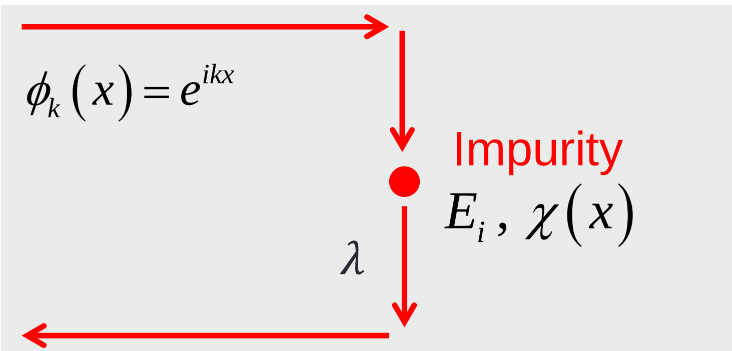
Antiresonance



- Two bound states (electron-like and hole-like)
- Antiresonances in transmission at the bound state energies
- Decreasing antiresonance width with increasing strip width L

Antiresonance: model

Scattering problem: $\psi(x)=\phi_k(x)+\int_{-\infty}^{\infty}G(x,x')V(x')\psi(x')dx'$



$$G_{TI}=\frac{-i}{\hbar v}\begin{pmatrix} e^{ik(x-x')}\theta(x-x') & 0 \\ 0 & e^{ik(x'-x)}\theta(x'-x) \end{pmatrix}$$

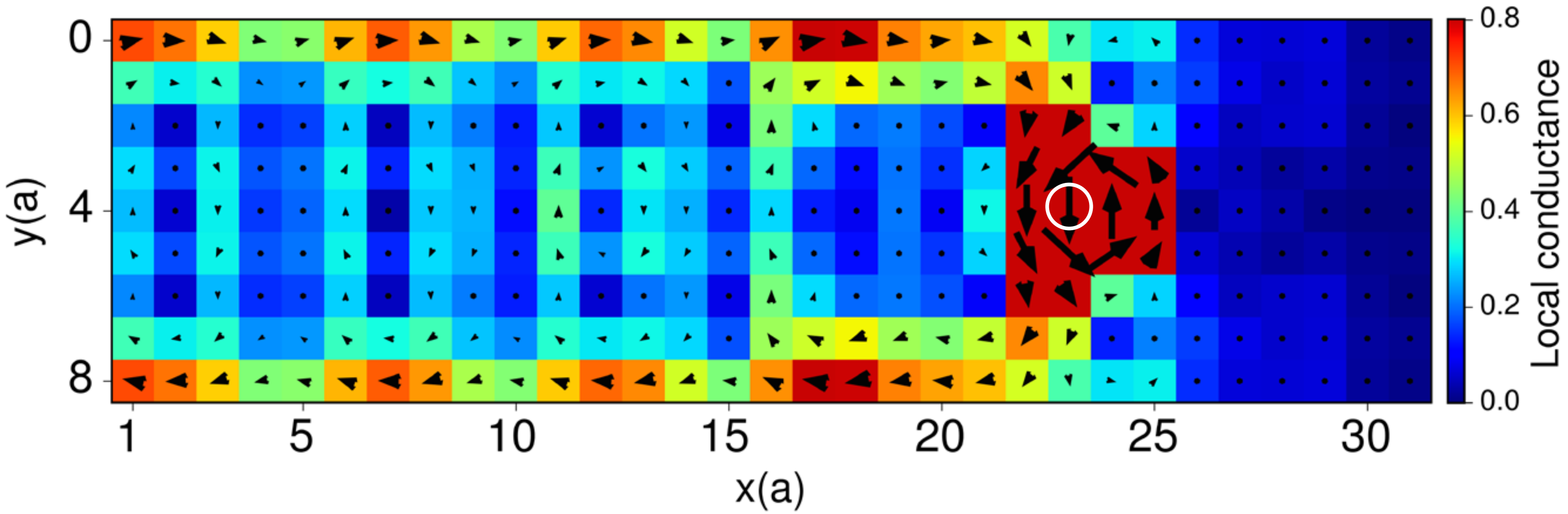
$$G_{imp}=\frac{\chi(x)\chi^*(x')}{E-E_i+i\eta}$$

Transmission: $T(E)=\frac{(E-E_i)^2}{(E-E_i)^2+\gamma^2}$

- Antiresonance in transmission characterized by width $\gamma=\frac{\lambda^2|\chi(0)|^2}{\hbar v}$

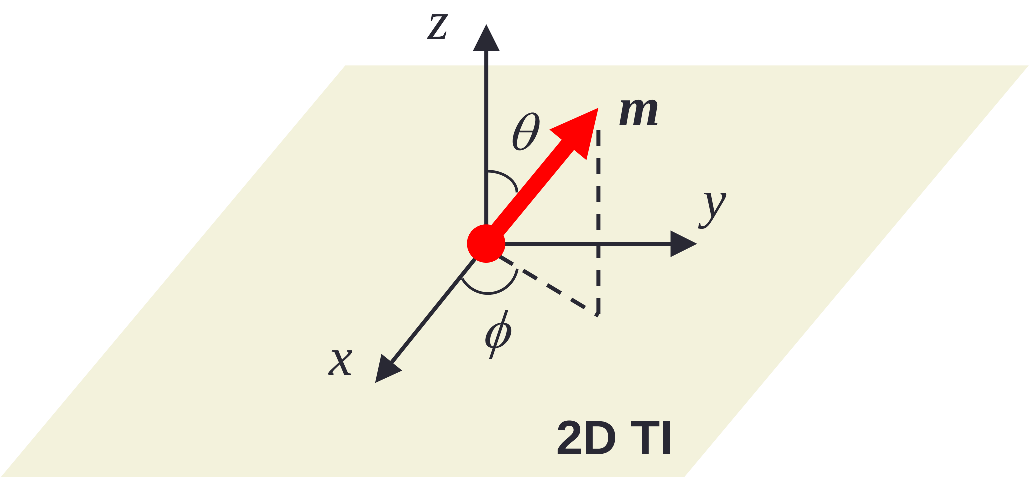
Antiresonance: local conductance

Spin up contribution



- Perfect back scattering due to antiresonance
- No net local currents
- Total transmission is zero

Effect of magnetic impurity



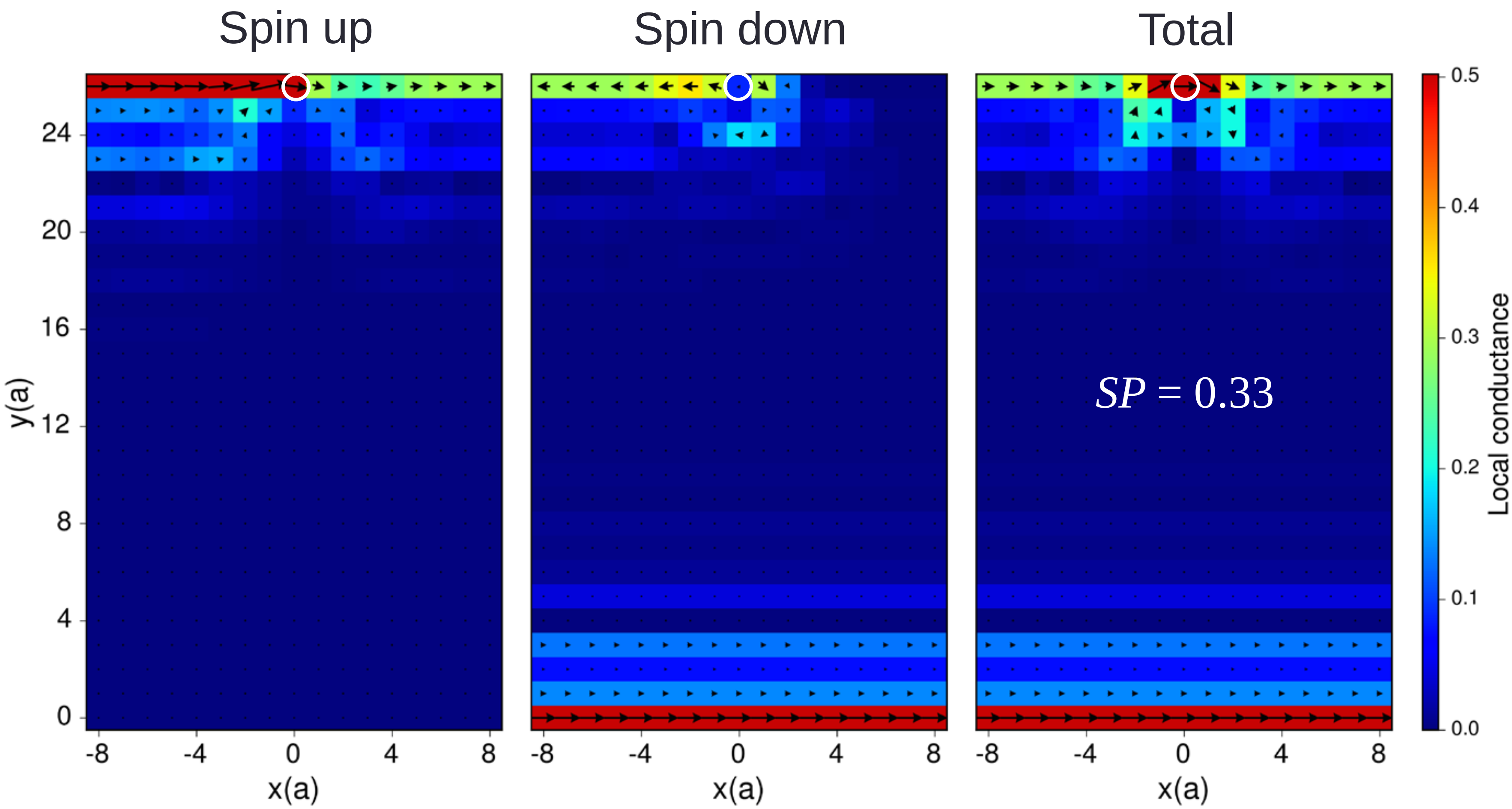
Magnetic impurity Hamiltonian:

$$H_{ex} = -\frac{\Delta}{2}\hat{m}\cdot\vec{\sigma}$$

$$\hat{m} = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta)$$

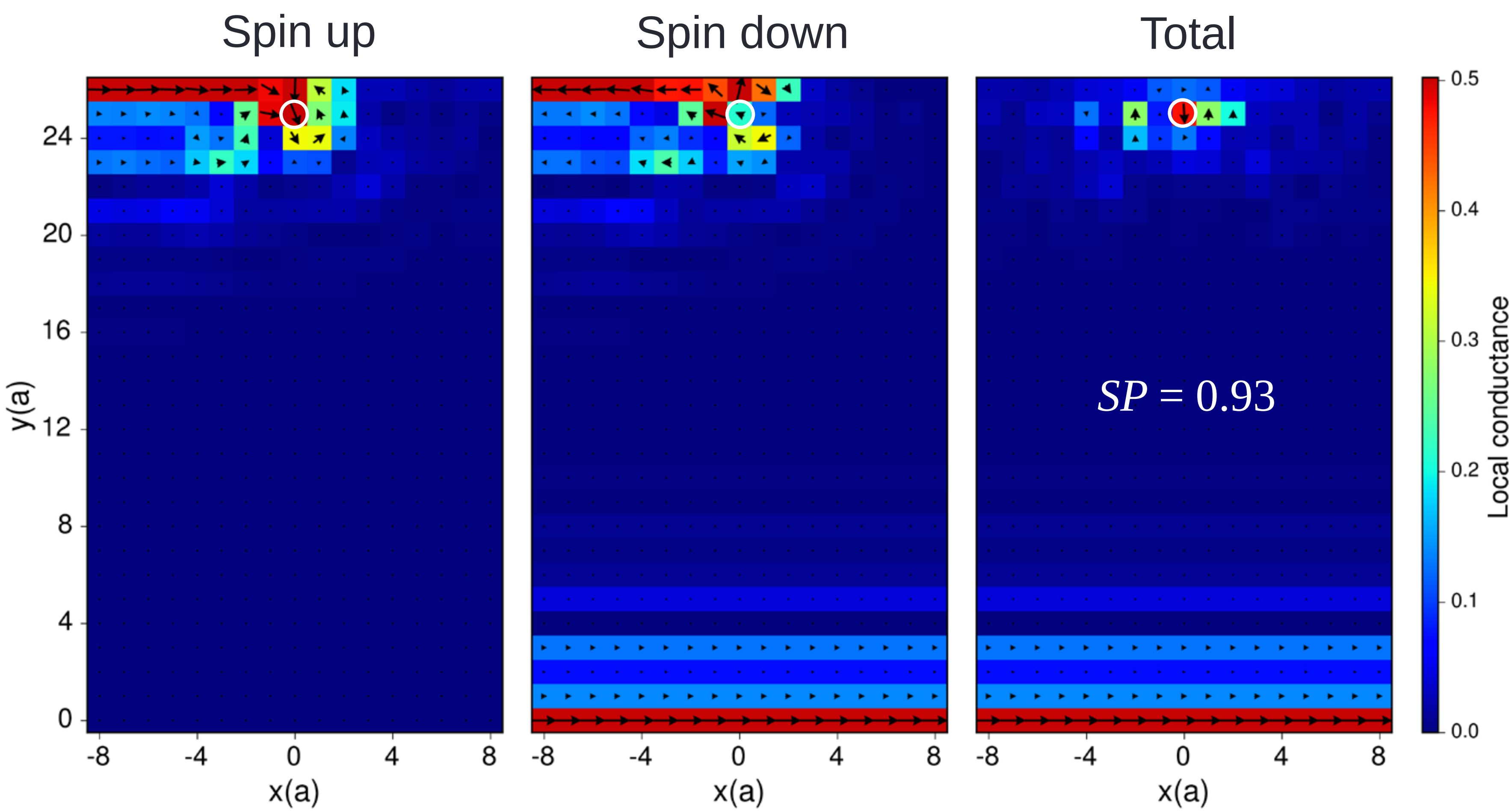
- ❑ Breaks time reversal symmetry
- ❑ Expected back-scattering due to mixing of spin channels
- ❑ Effect depends on the impurity magnetic moment angle
- ❑ Effect on transport spin polarization: $SP = \left|\frac{G_{\uparrow} - G_{\downarrow}}{G_{\uparrow} + G_{\downarrow}}\right|$

Magnetic impurity: local conductance



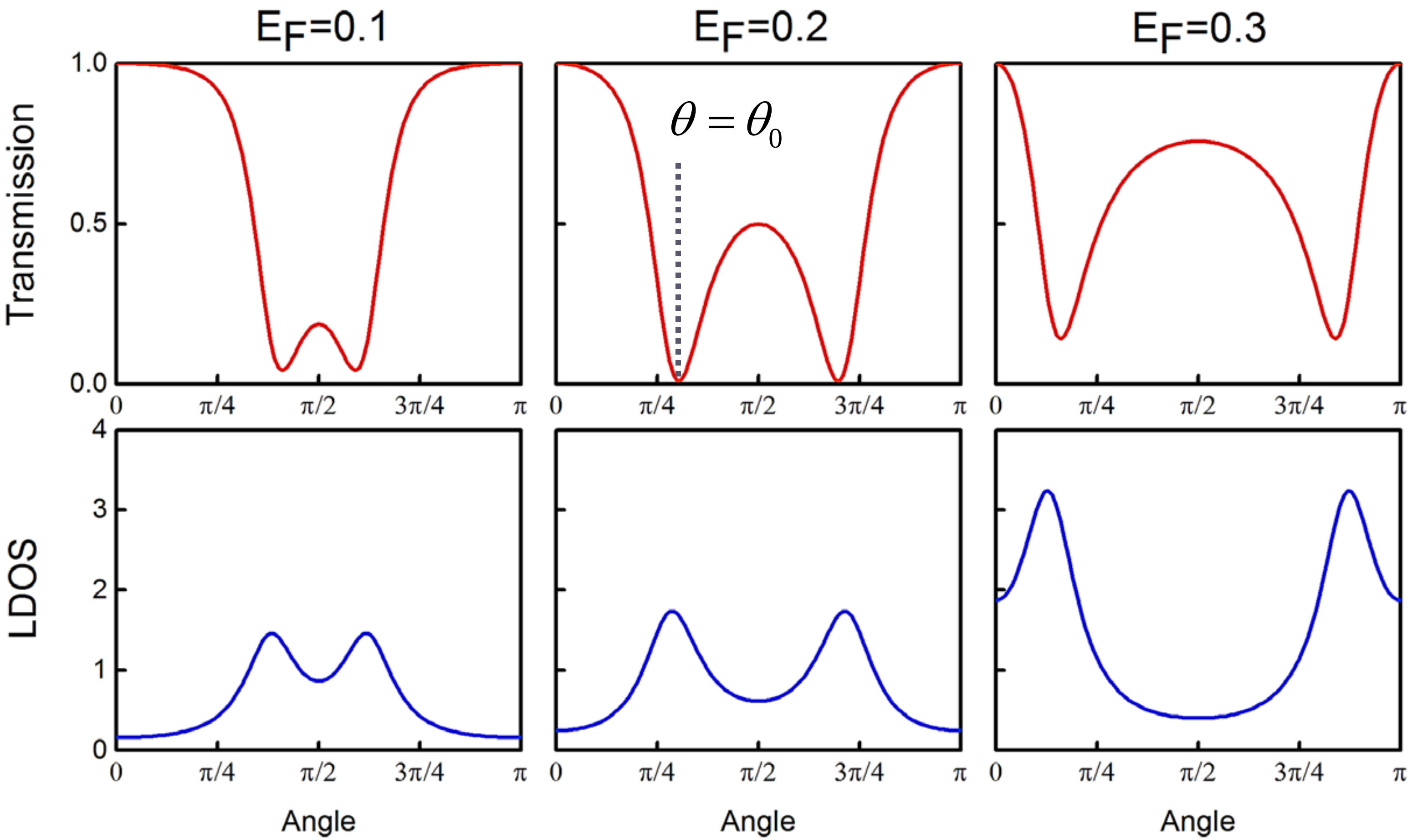
- Backscattering seen in spin-down channel

Magnetic impurity: local conductance



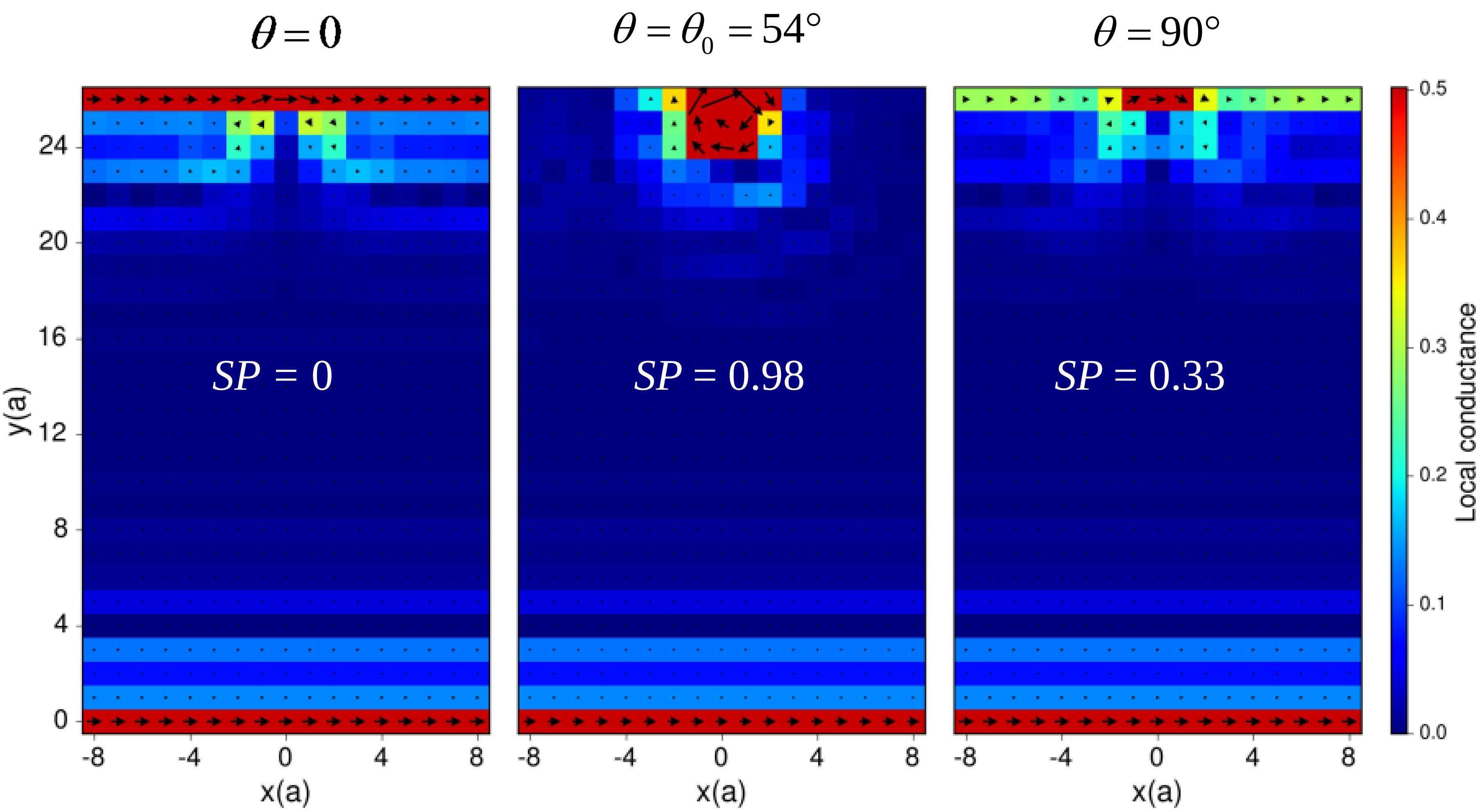
- Nearly perfect backscattering

Magnetic impurity: angular dependence



- Antiresonance in transmission due to magnetic impurity at the critical angle of the magnetic moment

Magnetic impurity: local conductance



- Current vertex at the antiresonance conditions

Summary

The BHZ model for a 2D topological insulator implemented within the tight-binding Green's function technique reveals:

- Oscillatory decay of the local conductance away from the TI edge
- Intricate current distributions and formation of current vertices of different chirality around impurities
- Oscillatory behavior of the edge-state energy gap as a function of 2D TI width
- Impurity-driven Friedel oscillations in electron density and spin-dependent local conductance for sufficiently narrow TI strips
- Resonant back scattering and antiresonances in transmission for finite-size impurity system
- Back scattering produced by magnetic impurity and resonant-type transmission as a function of magnetic moment angle