Unconventional transport in 2D materials with strong Rashba coupling

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Valuable discussions with:
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Phys. Rev. Lett. **116**, 166602 (2016)

Purpose of the talk

clarify whether and how spin-orbit coupling affects DC charge transport

Outline

- Motivations
- Model and regimes
- Results
  - Single-particle properties
  - Conductivity and mobility

  Simple analytical expressions !
- Perspectives

Spin-orbit (SO) coupling in solids

- weak anti-localization
- anomalous Hall effect
- spin Hall effect, spin relaxation
- topological phases
- Majorana fermions
-...

SPINTRONICS = spin transport electronics ⇒ "understand and control the transport of spin-polarized currents and to eventually apply this knowledge in information technologies"

D. Awshalom, Physics (2009)

Intense efforts to engineer structures and materials with strong spin-orbit coupling

Types of spin-orbit coupling

- Intrinsic
  - **Rashba** ⇐ structural inversion asymmetry or external gates
  - Dresselhaus ⇐ bulk inversion asymmetry
- Extrinsic → Due e.g to scattering with impurities...

In this talk: Rashba spin-orbit coupling in charge transport

Emerging new materials …

- Surface alloys

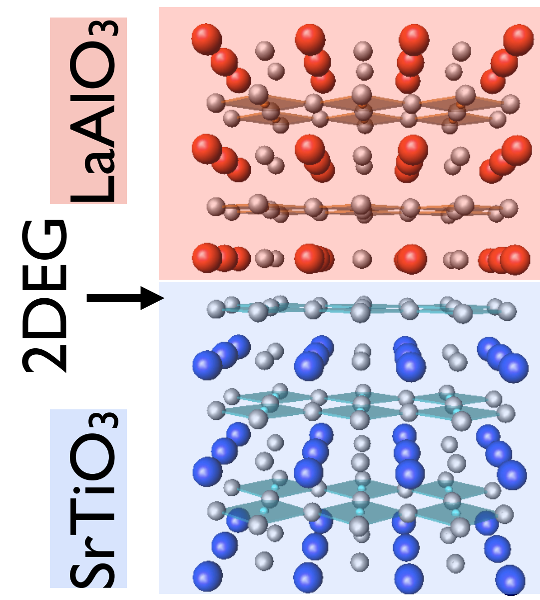
Adatoms: Bi, Pb

C. Ast *et al., Phys. Rev. Lett. (2007); K.Yaji et al., Nature Comms. (2009);*

Tunability by changing stoichiometry

Spin-orbit coupling up to 200 meV

- Oxides heterostructures

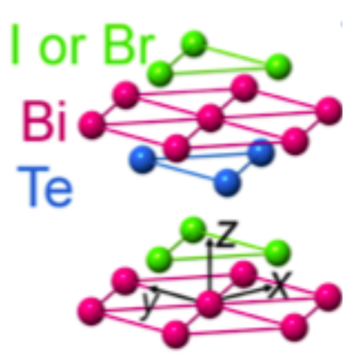


A. Ohtomo & . Huang, Nature (2004); A. Caviglia *et al., Nature* (2008); …

Gate tunable

Spin-orbit coupling estimates range from 5 to 20 meV;

- Surfaces of BiTeX, X=Cl,I,..



Spin-orbit coupling up to 100 meV

After Sakano et al. Phys. Rev. Lett. (2013); Eremeev et al.ibid. (2012); A. Crepaldi ibid. (2012);…

- Other systems:
  - HgTe quantum wells
  - Organometal compunds
  - Ferroelectric materials
  - …

…with strong (*tunable*) *Rashba* coupling

Common features are:

- 2-dimensional
- strong spin-orbit coupling, E_0
- tunable carrier density, small E_F

Very different from traditional III-V semicondutors where SO coupling is a small perturbation!

Need for a theoretical description of transport non-perturbative in E_0/E_F

Model

$$H = \int d\mathbf{r}\, \Psi^\dagger(\mathbf{r}) \left[\frac{p^2}{2m} + \alpha\, \hat{z} \cdot (\mathbf{p} \times \vec{\sigma}) + V_{\mathrm{imp}}(\mathbf{r}) \right] \Psi(\mathbf{r})$$

Rashba Hamiltonian + Disorder

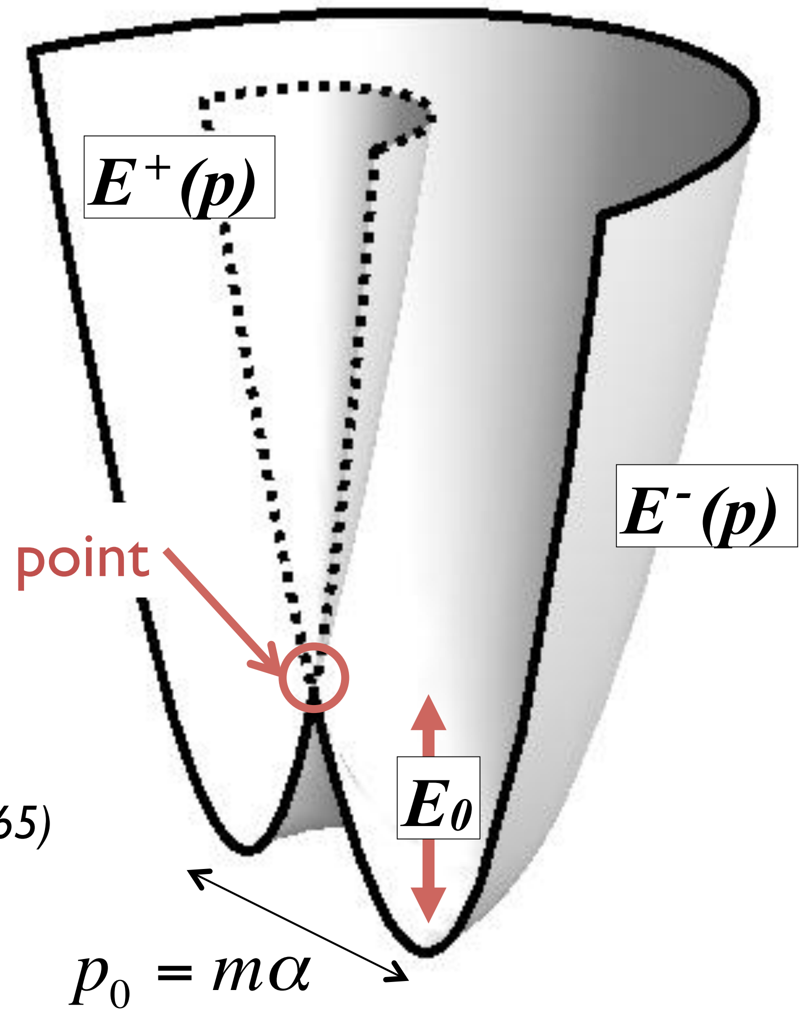
- **Rashba Hamiltonian** $H^{\mathrm{R}}_{\mathbf{p}} = \frac{p^2}{2m} + \alpha|\mathbf{p}|S$

Helicity: $S = [\hat{p} \times \vec{\sigma}]_z$ $S|\mathbf{p}s\rangle = s|\mathbf{p}s\rangle$ $s = \pm 1$

Two bands with opposite helicities $E^s(p) = \frac{p^2}{2m} + s\alpha\,|\vec{p}|$

Spin-orbit coupling strength:	$E_0 = \frac{m\alpha^2}{2}$

E.I. Rashba, *Sov. Phys. Usp. (1965)*



- **Disorder** due to static impurities with density n_i: $\langle V_{\mathrm{imp}}(\mathbf{r})V_{\mathrm{imp}}(\mathbf{r}')\rangle_{\mathrm{imp}} = n_i v^2_{\mathrm{imp}}\delta(\mathbf{r}-\mathbf{r}')$

Amount and strength of impurity scattering defined by:	$\Gamma_0 = \frac{m n_i v^2_{\mathrm{imp}}}{2}$	elastic scattering rate at zero SOC

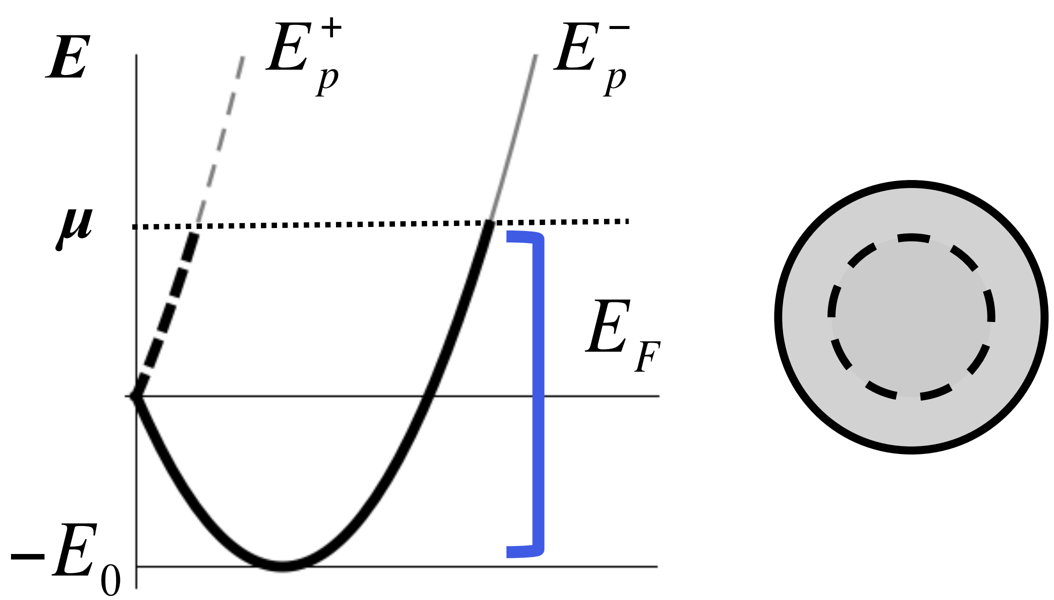
- Elastic s-wave scattering
- Inelastic scattering (phonons, e-e) negligible

Work on-going with Capone's group !

Two charge-transport regimes

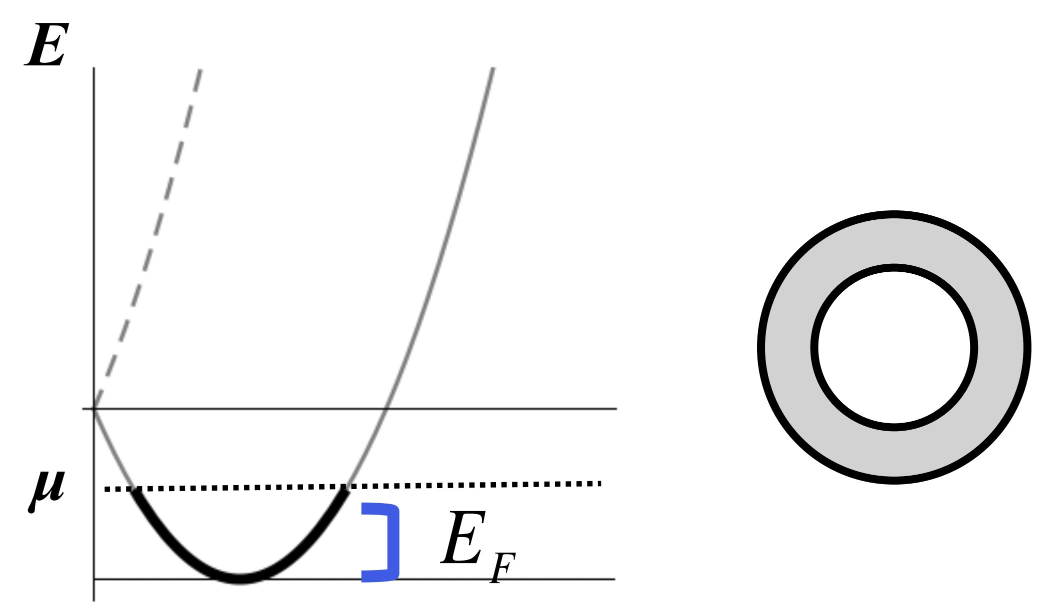
Relevant energy scales: Γ, E_0 and E_F Diluted impurities $\Rightarrow$ $\Gamma < E_F, E_0$

High-density (HD) regime : $E_F > E_0$



Fermi surface (FS) = two circles with opposite helicities

Dominant spin-orbit (DSO) regime: $E_F < E_0$

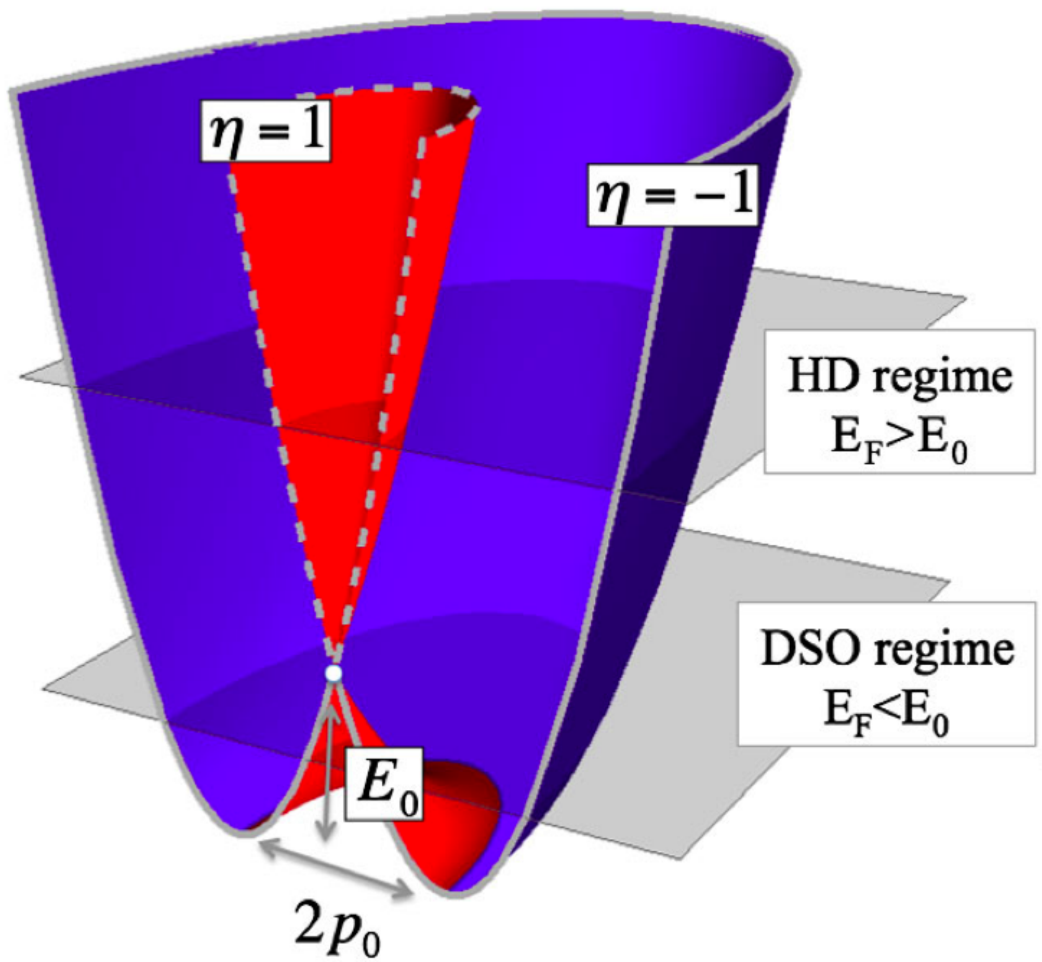


FS = two circles with equal helicities but opposite velocities

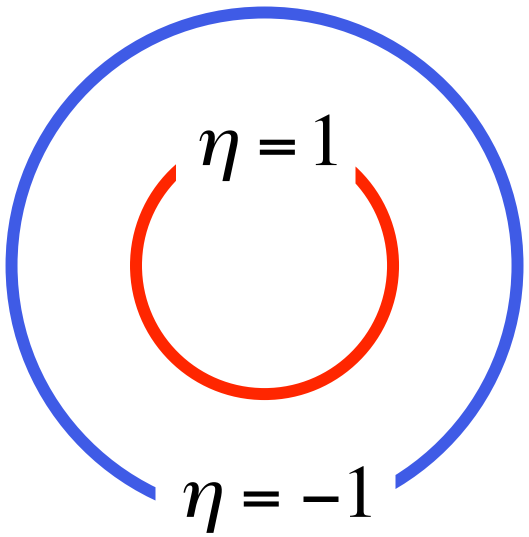
Sign-change in the quasi-particle velocity suggest a universal classification of the states in the two-regimes!

Transport helicity $\eta = (\hat{v}_{\mathbf{p}s} \cdot \hat{p})\, s$

Average velocity of helicity state s



In both regimes we have FS with opposite transport helicities:



- Unified classification of the states in the two regimes;
- Simple and compact description of transport.

To different eigenvalues of the transport helicity correspond very different transport properties!

Single-particle properties

Green's function

- Diagonal Green's function in the helicity basis

$$G^R(\mathbf{p},\omega) = \begin{pmatrix} g_+^R(p,\omega) & 0 \\ 0 & g_-^R(p,\omega) \end{pmatrix}$$

$$g_s^R(p,\omega) = \left[\omega - E_p^s + \mu - \Sigma^R(\omega)\right]^{-1}$$

- Spin-independent self-energy!

$$\Sigma^R(\omega) = \frac{n_i v_0^2}{\mathcal{V}} \sum_{\mathbf{p},s} g_s^R(p,\omega)$$

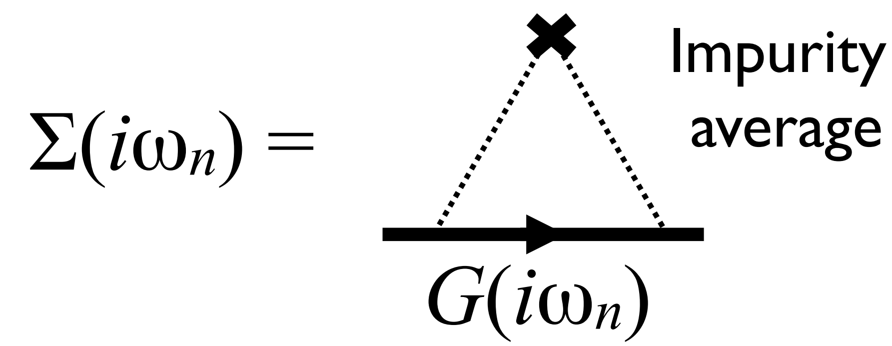
DOS and elastic scattering rate:

$$\left.\begin{matrix}\Gamma \\ N(E_F)\end{matrix}\right\} \propto -\mathrm{Im}\left[\Sigma^R(0)\right]$$

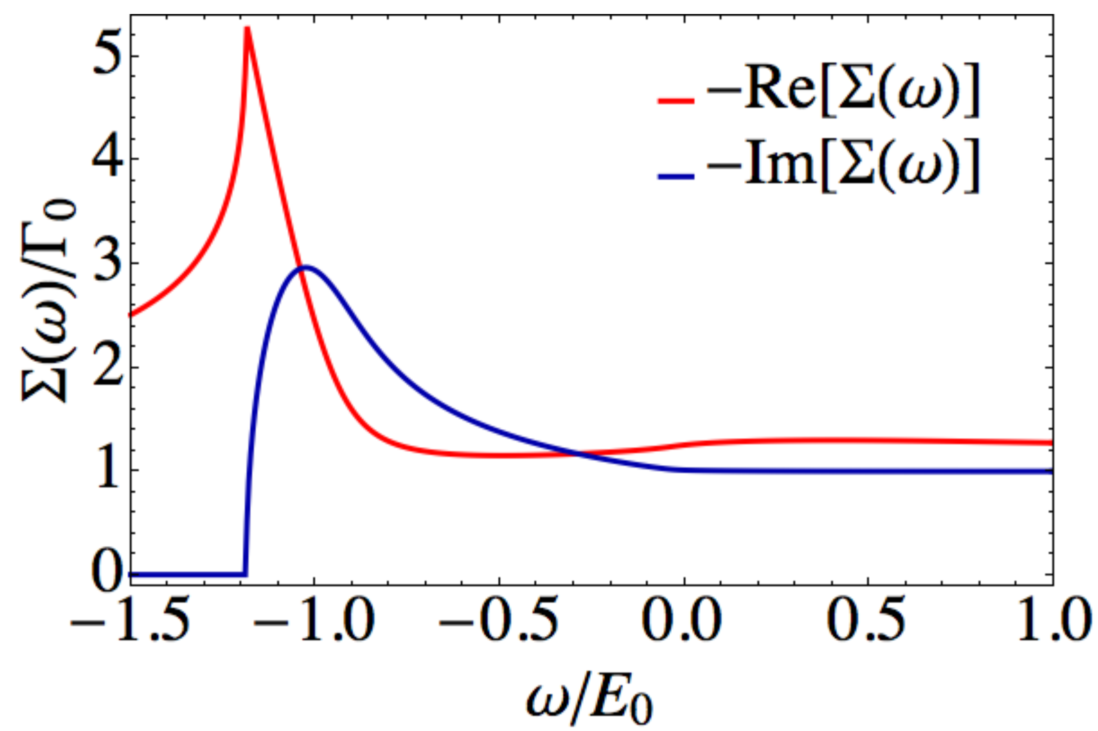
To lowest order in $\dfrac{\Gamma}{E_F}$

Diagrammatic perturbation theory in Matsubara frequencies

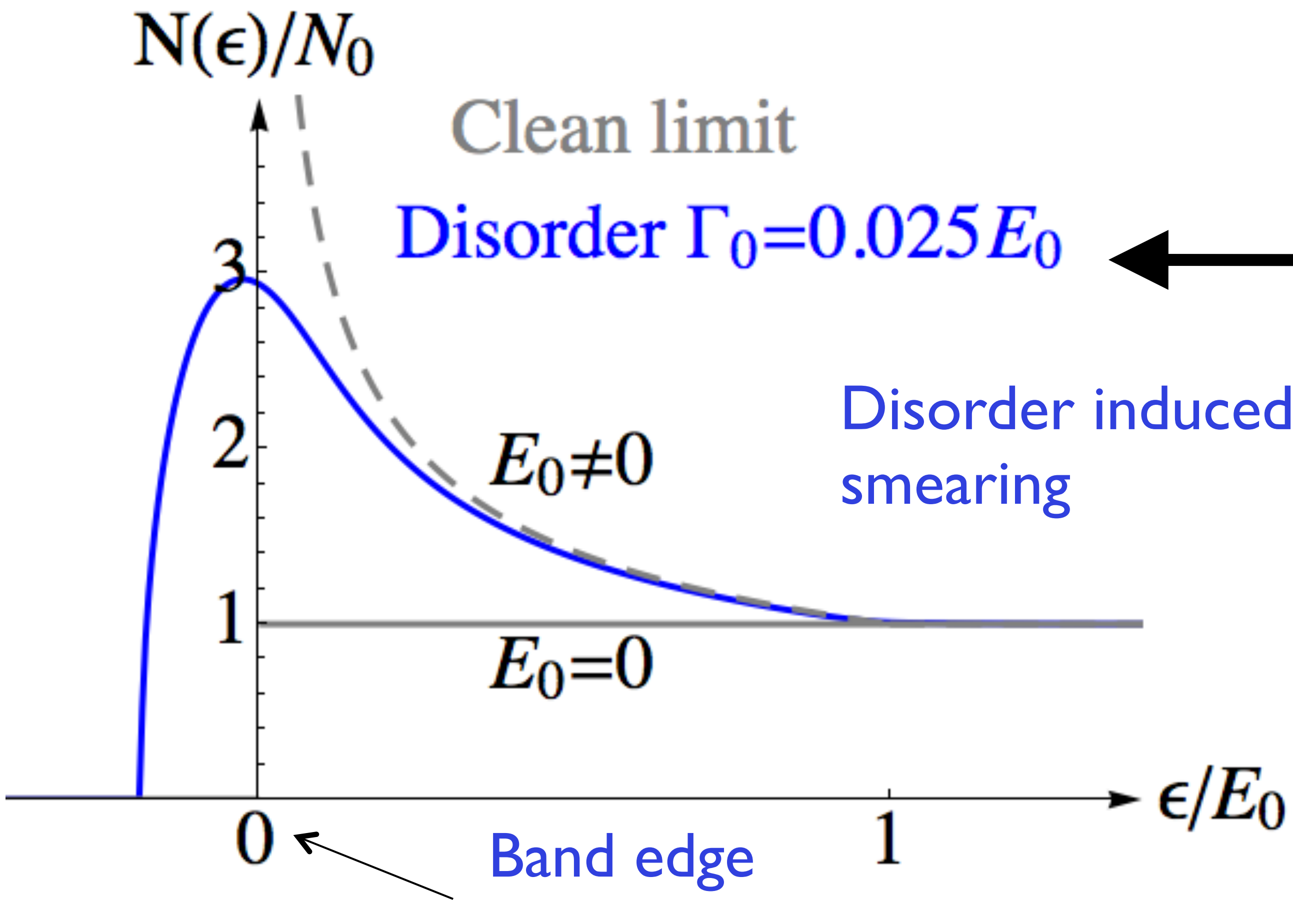
Self-consistent Born approximation (SCBA)



Self-consistency close to band-edge



Density of states (DOS)

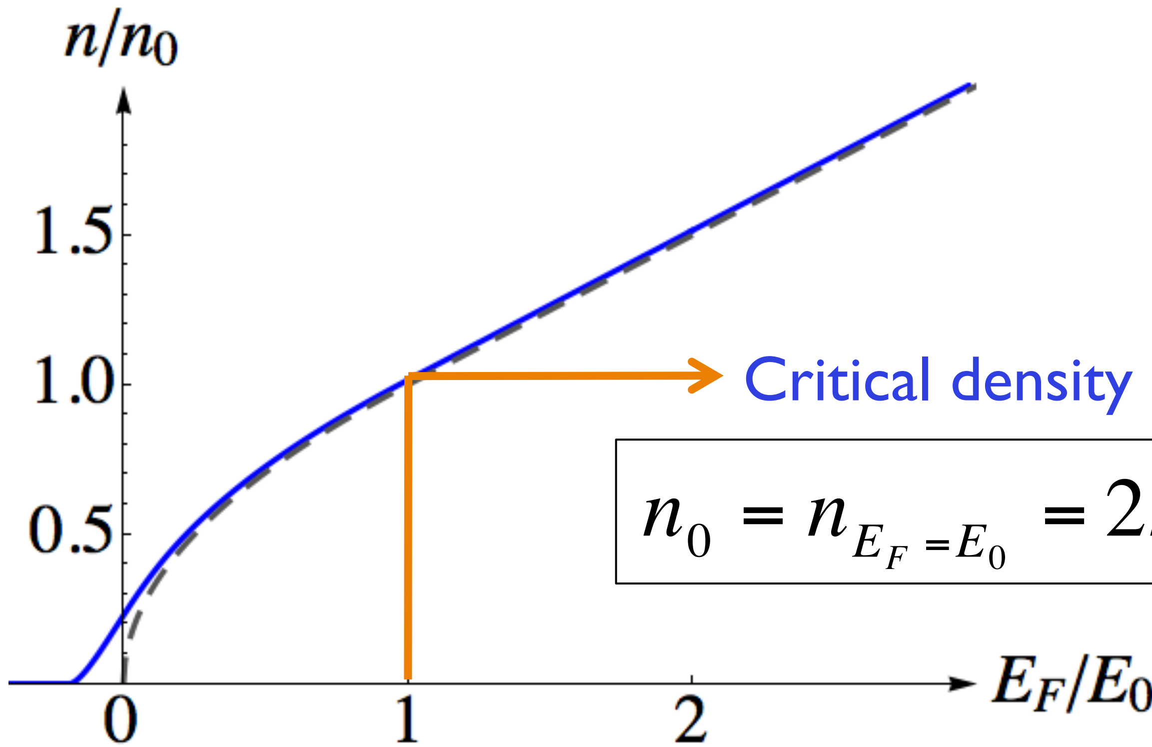


Van Hove singularity due to Rashba coupling

$$N(\varepsilon) = \begin{cases} N_0 & E_F > E_0 \\ N_0\sqrt{E_0/\varepsilon} & E_F < E_0 \end{cases}$$

$$N_0 = m/\pi$$

Charge density

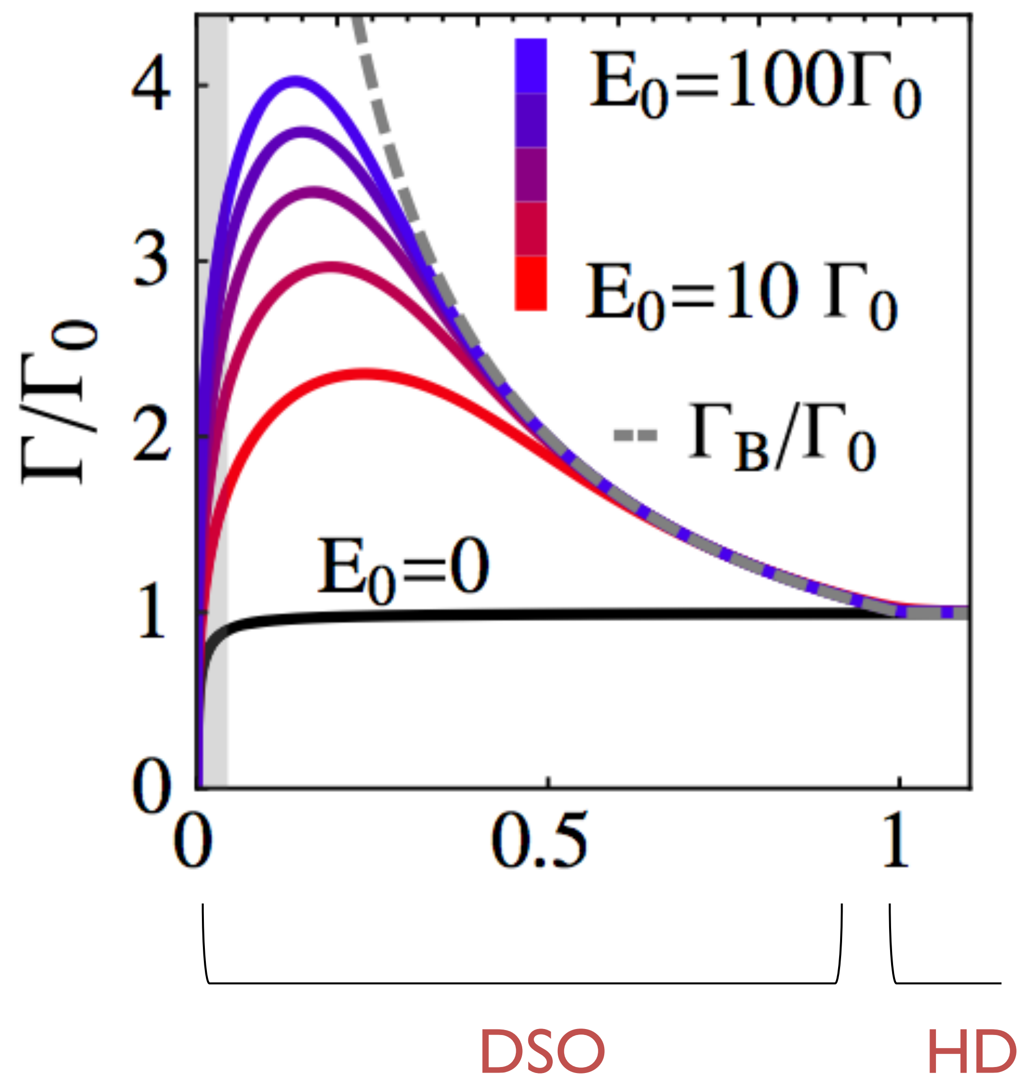


$$n_0 = n_{E_F = E_0} = 2mE_0/\pi$$

$$n = \begin{cases} N_0(E_F + E_0) & E_F > E_0 \\ 2N_0\sqrt{E_F E_0} & E_F < E_0 \end{cases}$$

Analytical formulae in clean limit !

Elastic scattering rate



Shaded region : corrections to SCBA important

Van Hove singularity → Clearly different behavior in the HD and DSO regimes!

⇔ Neglect broadening of spectral functions

$$|g_s^R(p,0)|^2 \simeq \delta(E_p^s - \mu)\pi/\Gamma$$

Well-defined quasi-particles

Fully quantum approach ⇔ Boltzmann approach

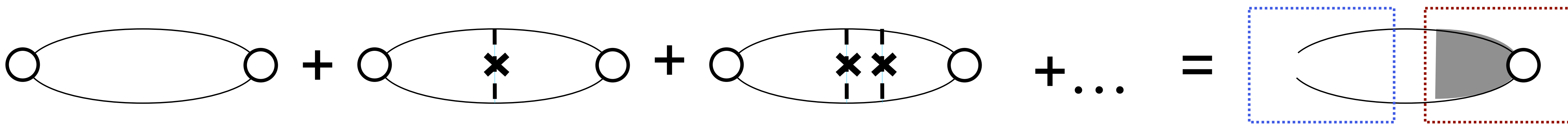
Simple analytical formulae

HD regime : $\Gamma_B \cong \Gamma_0$ → $\tau \cong \tau_0$

DSO regime: $\Gamma_B \cong \Gamma_0 \dfrac{n_0}{n}$ → $\tau \cong \tau_0 \dfrac{n}{n_0}$

Transport properties

Kubo formula



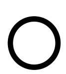
Matsubara frequencies diagrams

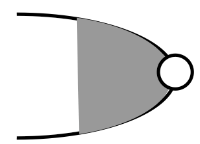
Bare current

"Dressed" current

$$\sigma \simeq \frac{1}{2\pi\mathcal{V}} \sum_{\mathbf{p}} \mathrm{Tr}\left[j_x(\mathbf{p}) G^R(\mathbf{p},0) J_x^{RA}(\mathbf{p}) G^A(\mathbf{p},0)\right]$$

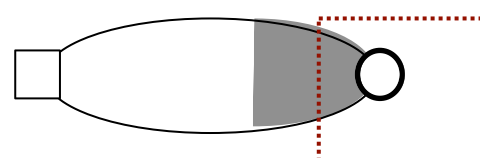
A or R = advanced or retarded argument

 = $j_x(\mathbf{p}) = e(p_x/m + \alpha\sigma_y)$

 = $J_x^{RA}(\mathbf{p}) = e(p_x/m + \tilde{\alpha}^{RA}\sigma_y)$

Same vertex also leads to vanishing spin-Hall effect !!!

Spin-Hall bubble



Only the "anomalous" current is renormalized

Boltzmann approach: $\sigma_{\mathrm{dc}}^B = \frac{e^2 v_F}{4\pi} \sum_\eta \tau_\eta^{\mathrm{tr}} p_\eta = \sum_\eta \sigma_\eta$

Incoherent sum of contributions of the two FS corresponding to different η

Transport scattering times ← τ_η^{tr}

Fermi momenta : $p_\eta = |m v_F - \eta p_0|$ $\quad v_F = \sqrt{2mE_F}$

Conductivity

In the absence of spin-orbit coupling
within our assumptions:

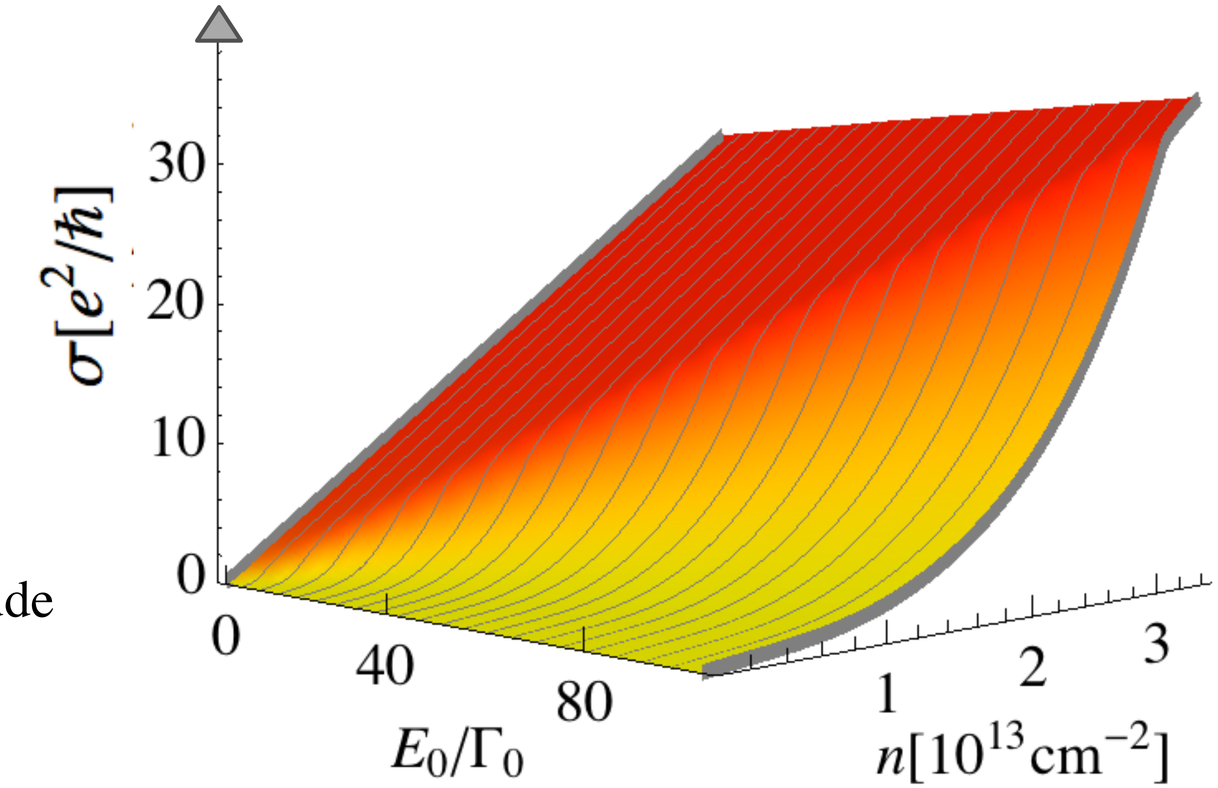
$$\sigma = \sigma_{\text{Drude}} \equiv \frac{e^2 n \tau}{m}$$

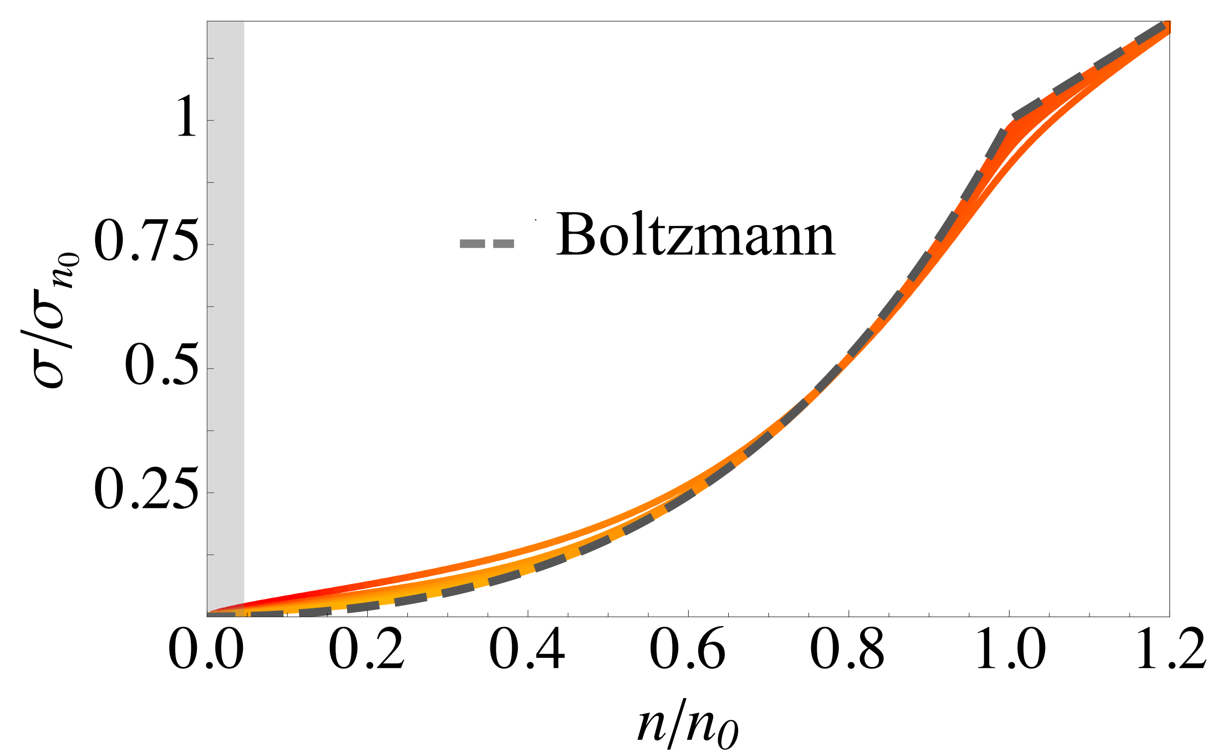
Conductivity as a function of density and Rashba coupling

$\sigma = 0$ $\qquad$ $\sigma = \sigma_{\mathrm{Drude}}$

$$\sigma_{\mathrm{Drude}} \equiv \frac{e^2 n \tau}{m}$$

- If $E_0 > \Gamma_0$ at low-doping conductivity becomes sublinear and deviates from Drude law
- By appropriate rescaling universal behavior obtained





Two charge-transport regimes

Analytical results within the approximation of well-defined quasi-particles

$n > n_0 \Rightarrow \sigma_{\mathrm{Drude}} \equiv \frac{e^2 n \tau}{m}$ $\qquad \tau \simeq \tau_0$

$n < n_0 \Rightarrow \sigma_{\mathrm{DSO}} \equiv \frac{e^2 n_0 \tau_0}{2m}\left(\frac{n^2}{n_0^2} + \frac{n^4}{n_0^4}\right)$ $\qquad \tau \simeq \tau_0 \frac{n}{n_0}$

Remarkably simple formula!

In both cases coincide with Boltzmann results!

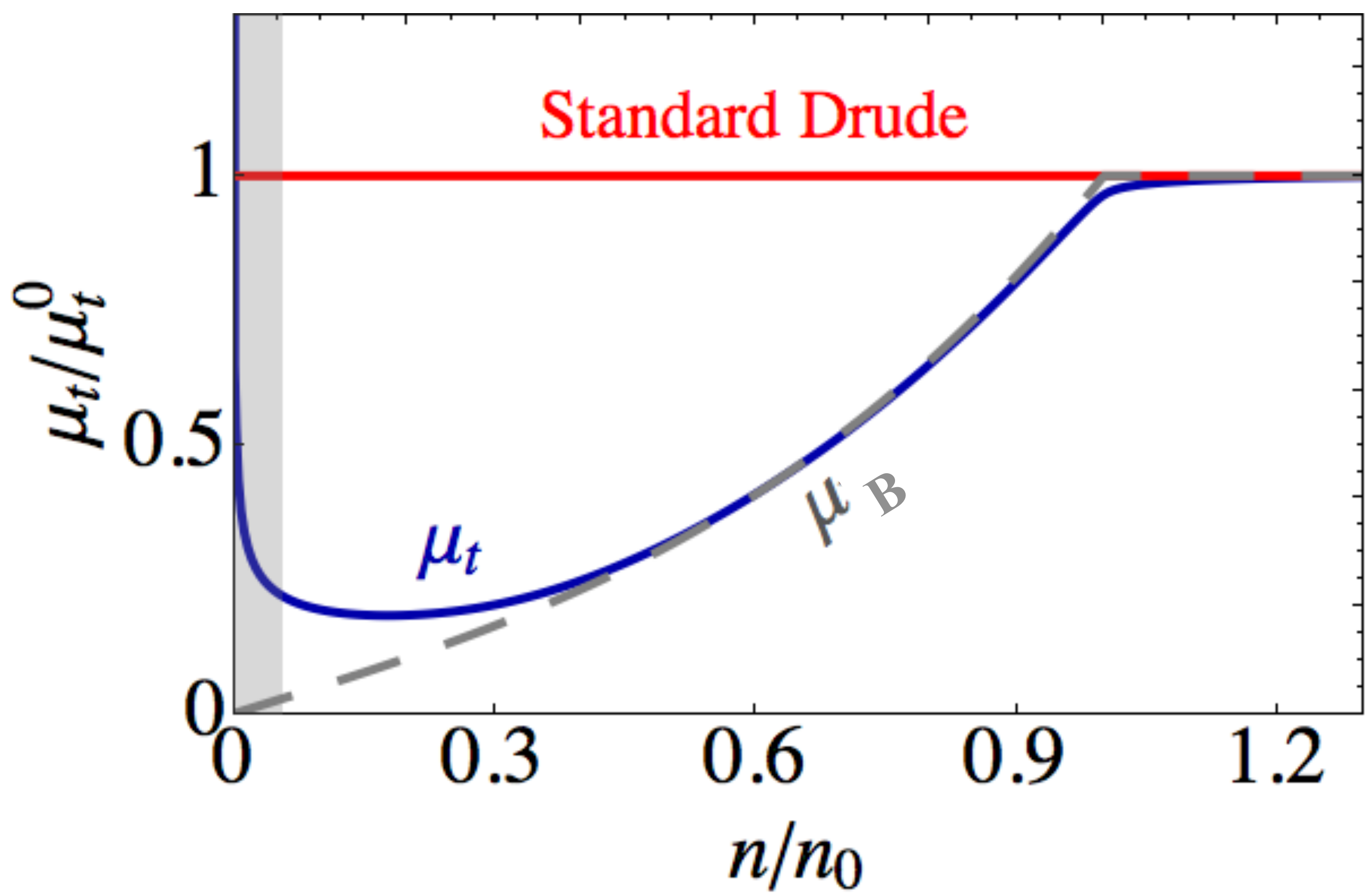
Decrease of the conductivity due to BOTH

- Increase of the scattering rate
- Non-zero anomalous vertex

$$\sigma_{\mathrm{DSO}} = \frac{1}{2}\left(1 + \frac{n^2}{n_0^2}\right)\sigma_{\mathrm{Drude}}$$

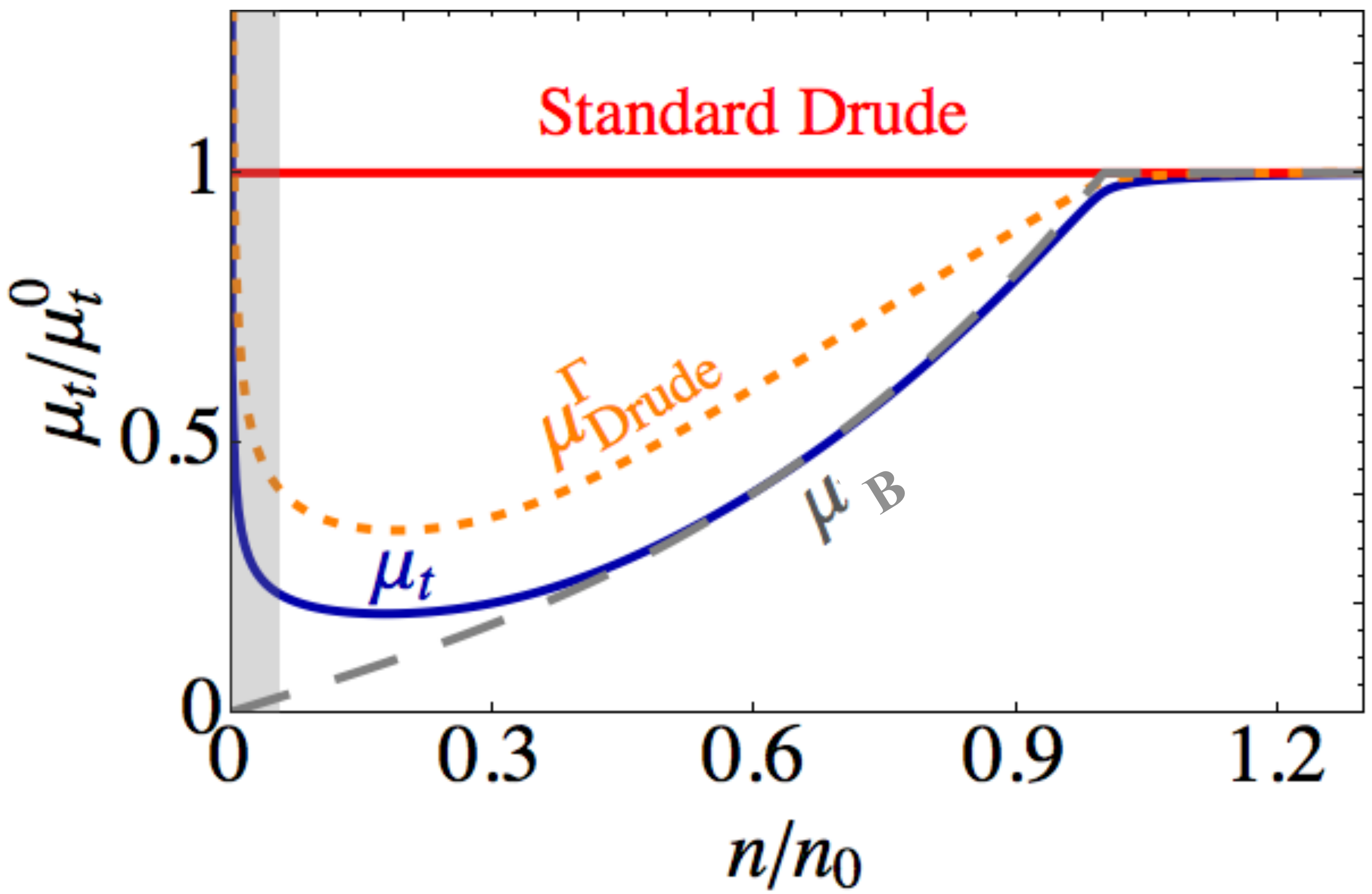
Mobility, μ_t Drift velocity per unit electric field $\mu_t = v_{drift}/E$

Related to the conductivity, *via* $\mu_t = \dfrac{\sigma}{en}$ Drude limit $\mu_t^0 = \dfrac{e\tau_0}{m}$



High accuracy of Boltzmann !

Two-fold origin mobility modulation



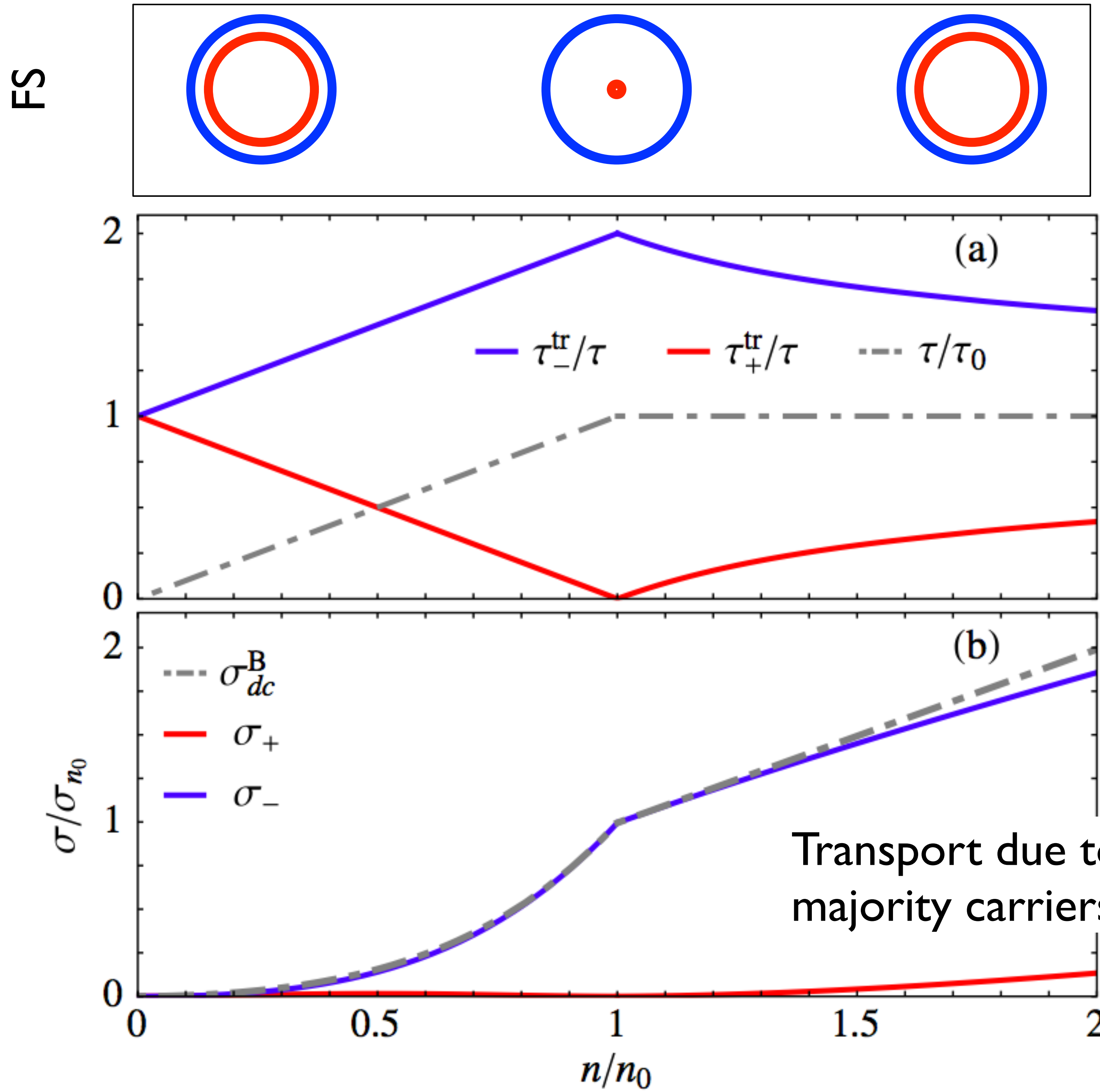
$$\mu^{\Gamma}_{\mathrm{Drude}} = \frac{e\tau}{m}$$

Strong dependence of the mobility on doping due to BOTH

- Increase of the scattering rate
- Non-zero anomalous vertex

Two types of charge carriers

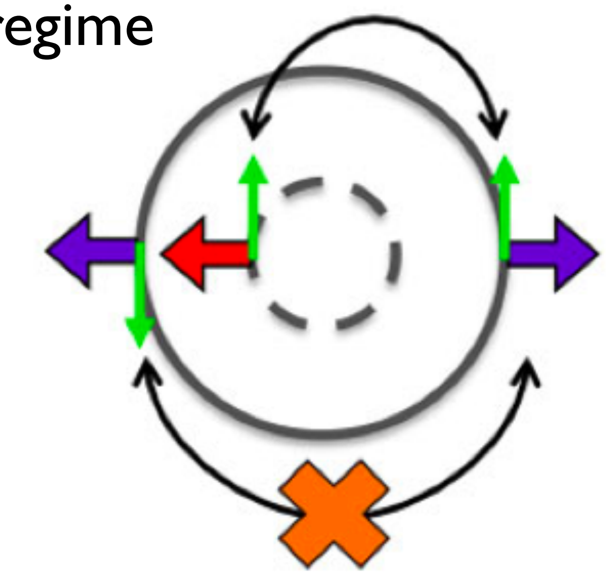
Different transport properties across different density regimes



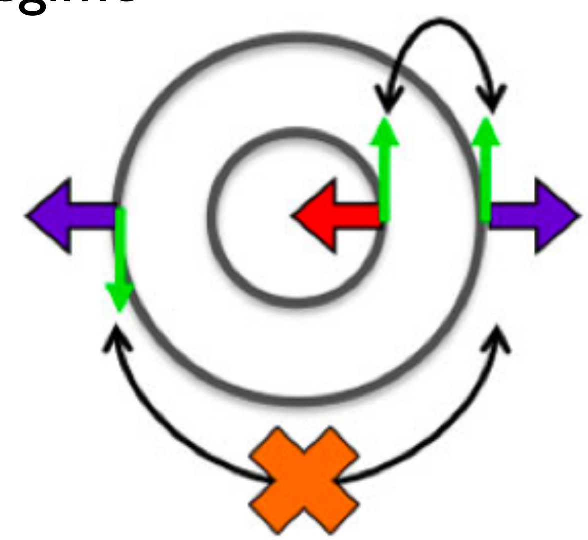
Transport due to majority carriers !

Suppression of backscattering within the same chiral band

HD regime



DSO regime



Conclusions

- In the HD regime: no effect of SOC on transport !!!

- In the DSO regime:

Van-Hove singularity Non-zero anomalous vertex	→	Reduction of the mobility and of the longitudinal conductivity

Analytical universal formulae to describe the conductivity which could be readily used to fit experiments

- Measure E_0 in a plain DC transport experiment!
- Use Rashba to control DC transport

ON-GOING WORK: EFFECT OF RASHBA SPIN-ORBIT COUPLING IN STRONGLY CORRELATED ELECTRONIC SYSTEMS

In collaboration with:
A. Amaricci, M. Capone and L. Fanfarillo @ SISSA
G. Sangiovanni @ Wurzburg