Diffusion of Dirac fermions

P. Adroguer

Laboratoire de Physique, Ecole Normale Supérieure de Lyon, France

ENS DE LYON

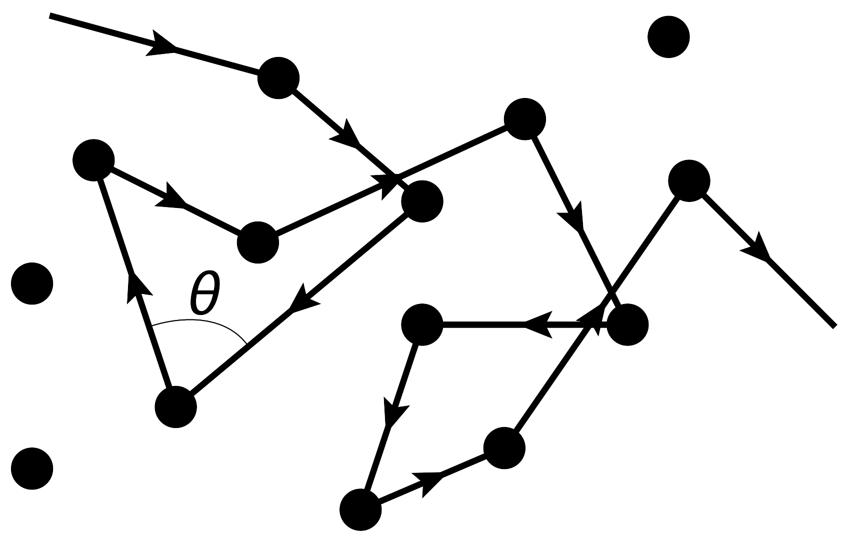
Outline

- Diffusion, regime of weak disorder
- Diffusion of Dirac fermions
    - 3D Strong topological insulators
    - Graphene
- Diffusion of semi-Dirac excitations

Outline

- Diffusion, regime of weak disorder
- Diffusion of Dirac fermions
    - 3D Strong topological insulators
    - Graphene
- Diffusion of semi-Dirac excitations

Diffusion



- Continuity limit of a random walk (mean free path l_e)
- Semi classical approach $\lambda_F \ll l_e$
- Experimental regime, high Fermi energy : good metal
- Sample length $\gg$ mean free path l_e
- Weak disorder regime

  - Boltzmann equation
  - Diagrammatics

Boltzmann equation

- Integro-differential equation

$$-e\vec{E}.\frac{\partial f}{\partial \vec{k}} = \langle \int \frac{d\vec{k'}}{(2\pi)^2} \quad 2\pi |\langle \vec{k'}|V|\vec{k}\rangle|^2 \delta(E(\vec{k'}) - E_F) \left[f(\vec{k'}) - f(\vec{k}) \right] \rangle$$

- 2 quantities of interest : scattering probability and density of states

- Linear response : Drude's conductivity (no quantum corrections, no UCF)

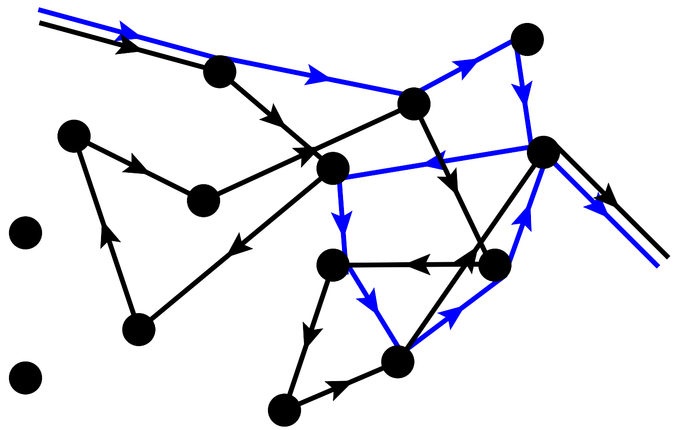
Standard diagrammatic technique

- Linear response : Kubo formula

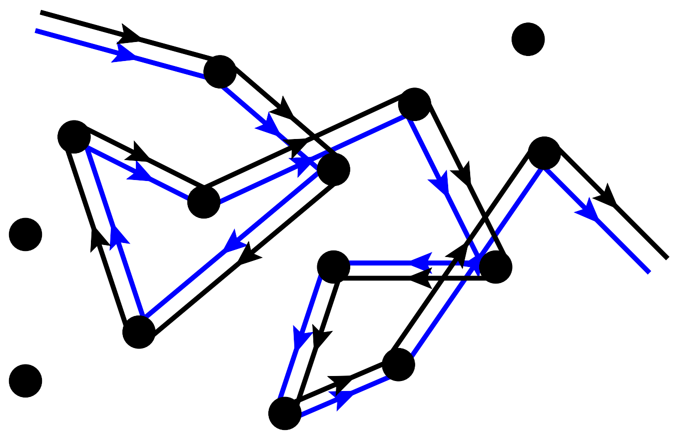
$$\sigma_{\alpha\beta} = \frac{\hbar}{2\pi\Omega} \Re\, Tr\left(j_\alpha G^R j_\beta G^A\right)$$

- Quantum mechanics

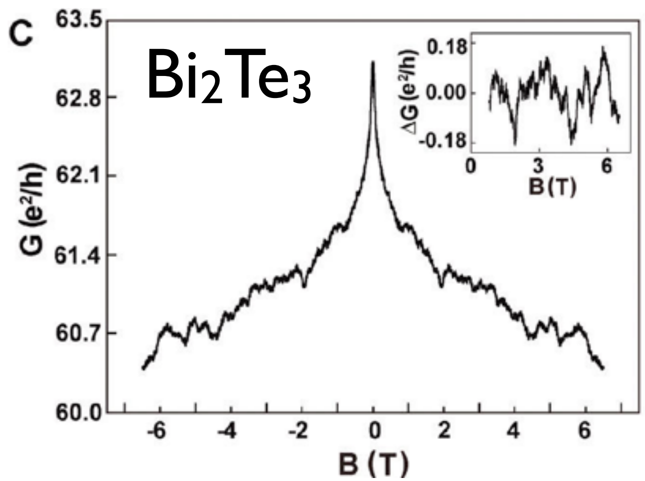
$$\sigma \propto \sum_{i,j} a_i^* a_j$$



- Classical part (diffuson) = Drude's conductivity



- Quantum interferences (cooperon) : WL, UCF



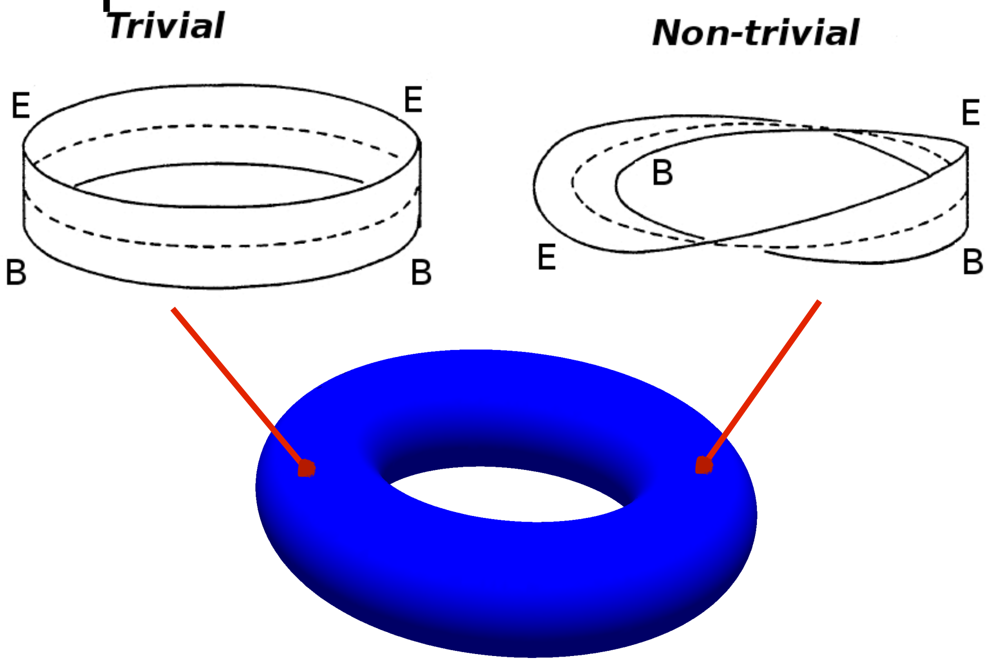
Kong et al. , 2010

Outline

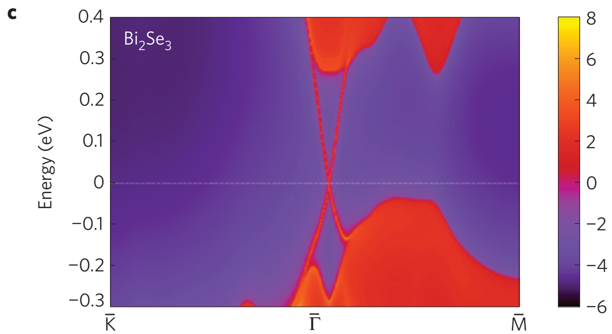
- Diffusion, regime of weak disorder
- Diffusion of Dirac fermions
    - 3D Strong topological insulators
    - Graphene
- Diffusion of semi-Dirac excitations

3D Strong topological insulators

- Insulators with topologically protected surface states

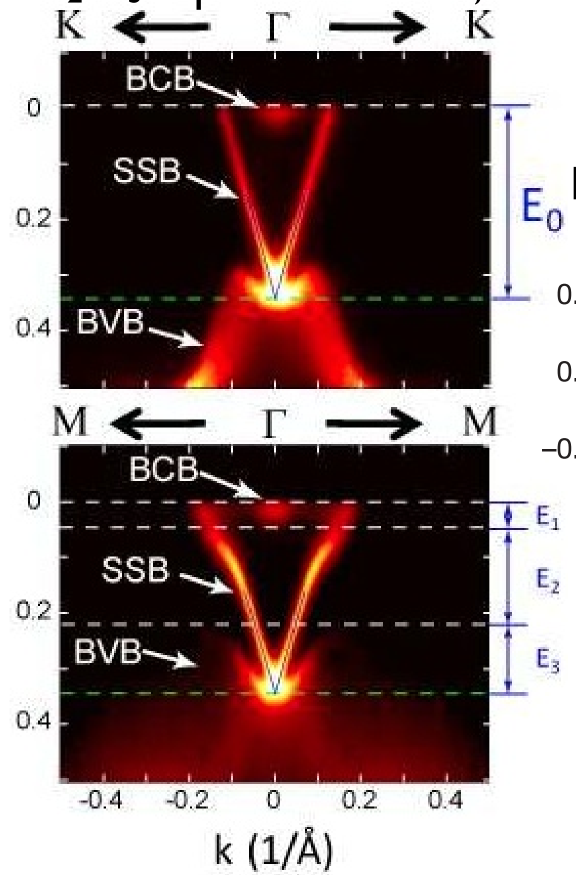


- Numerical simulations

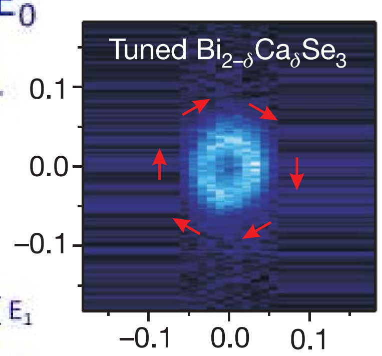


- Surface experiments (ARPES, STM)

Bi_2Te_3 Alpichshev *et al.* ,2010



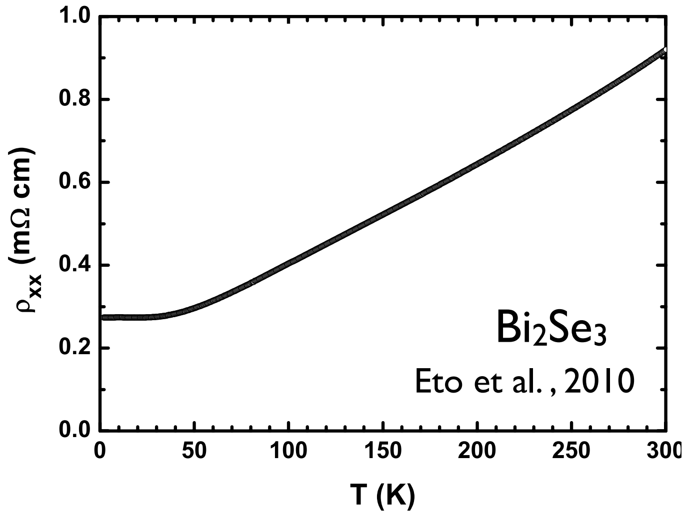
D. Hsieh *et al.* , 2009



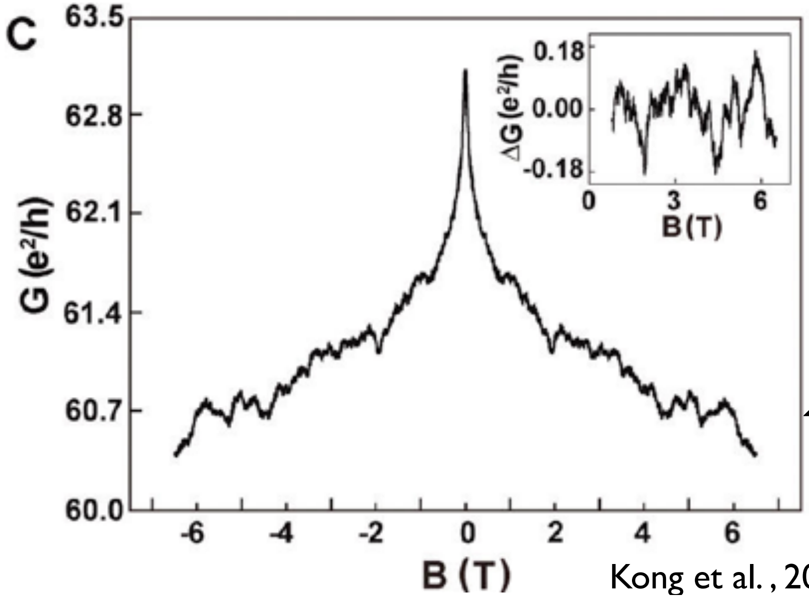
- Surface states : Odd number of Dirac cones

3DTI Transport experiments

- Residual bulk conductance
  - Thin films : improve surface/bulk ratio, gating both surfaces
  - Strained HgTe : no bulk conductance



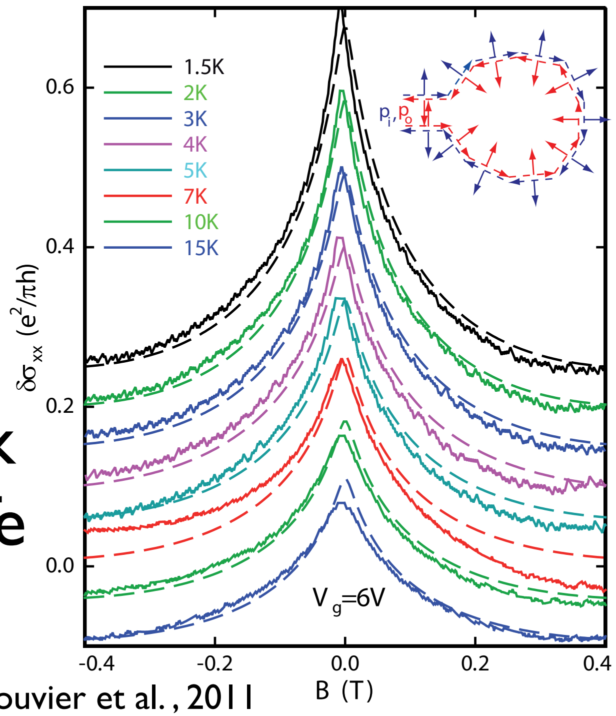
- Magneto-transport : weak anti-localization



Bi_2Te_3 thin film

Kong et al. , 2010

Bulk HgTe



Bouvier et al. , 2011

Regime of diffusive transport

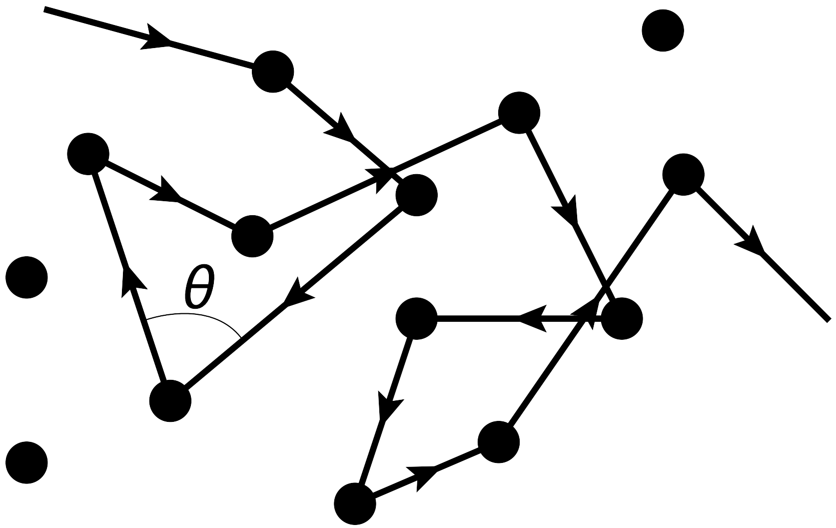
- Semi classical approach, $\lambda_F \ll l_e$ (perturbative approach)
- Experimental regime : far from the Dirac point (good metal)
- Hamiltonian : $\mathcal{H} = \hbar v_F \left(\vec{k} \times \vec{\sigma} \right) .\hat{z} + V(\vec{r})$

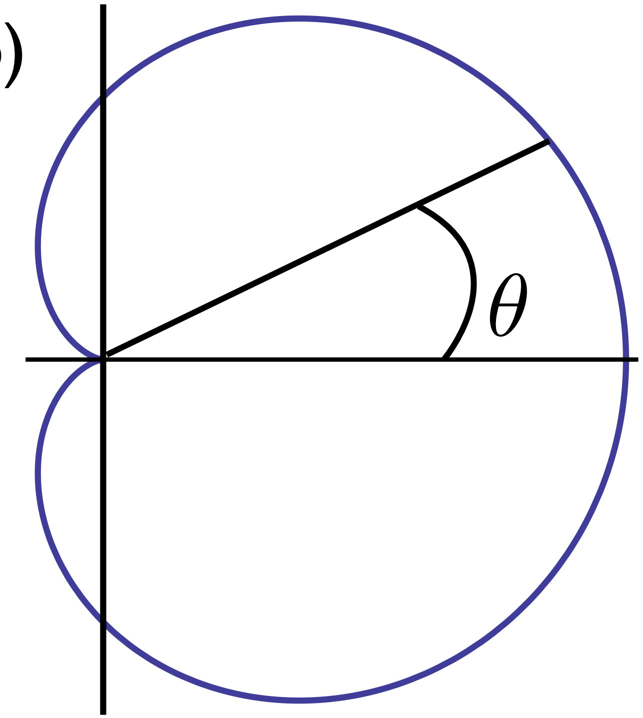
$$\langle V(\vec{r}) \rangle = 0 \qquad \langle V(\vec{r}) V(\vec{r'}) \rangle = \gamma \delta(\vec{r} - \vec{r'})$$

- Sample length $\gg$ mean free path l_e
- Weak disorder regime

Boltzmann equation

- Scattering anisotropy (spinor overlap)





- Absence of backscattering (TRS)
- Doubling of the transport time

$$\sigma = \frac{e^2}{h}\rho(E)v_F^2\tau_e \qquad D = v_F^2\tau_e = \frac{v_F^2\tau_{tr}}{2}$$

Diagrammatic approach

- Diffuson spinorial structure

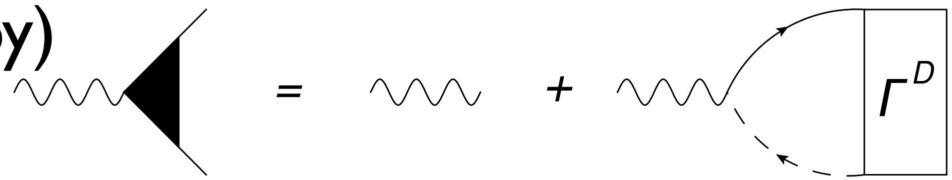
$$\Gamma^D(\vec{q}) = f_S(\vec{q})\ |S\rangle\langle S| + f_1(\vec{q})\ |T_1\rangle\langle T_1| + f_2(\vec{q})\ |T_2\rangle\langle T_2| + f_3(\vec{q})\ |T_3\rangle\langle T_3|$$

- One single diffusive mode :

$$\Gamma^D(\vec{q}) = \gamma \frac{1}{Dq^2\tau_e}\frac{1}{4}\left[Id \otimes Id + \sigma^x \otimes \sigma^x - \sigma^y \otimes \sigma^y + \sigma^z \otimes \sigma^z\right]$$

- Current operator renormalization (scattering anisotropy)

$$J_\alpha = 2 j_\alpha$$

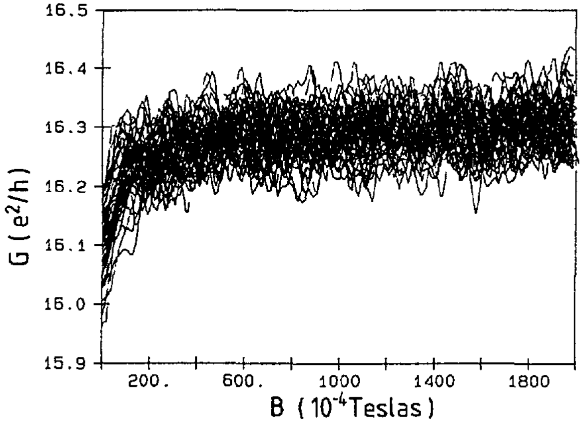


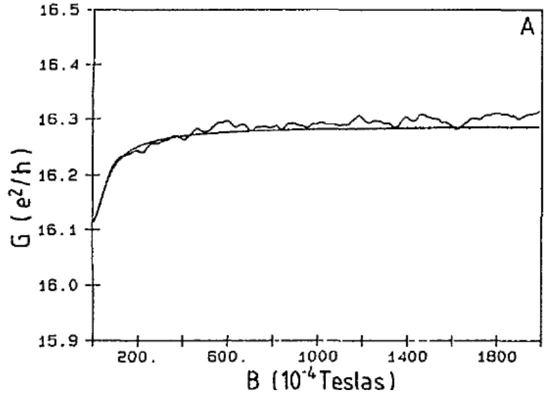
$$\sigma = \frac{e^2}{h}\rho(E) v_F^2 \tau_e \qquad D = v_F^2 \tau_e = \frac{v_F^2 \tau_{tr}}{2}$$

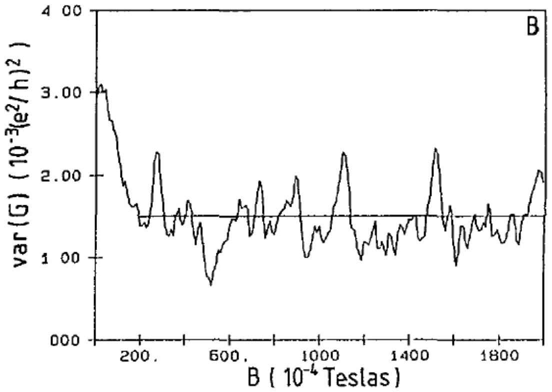
Doubling of transport time from anisotropy

Coherent transport

- Universal values : weak (anti)localization / UCF



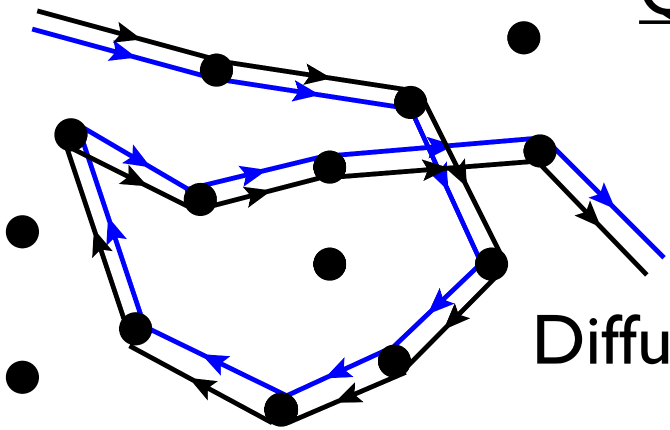




- Inelastic scattering : finite coherence time τ_φ

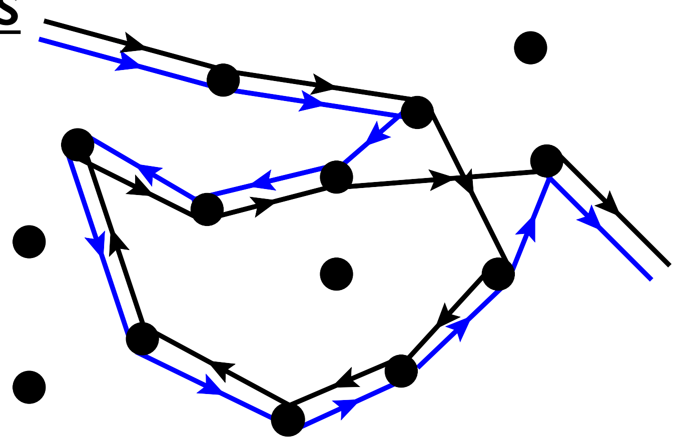
  Mesoscopic physics : low T ($\tau_\varphi \nearrow$), small samples

<u>Quantum interferences</u>



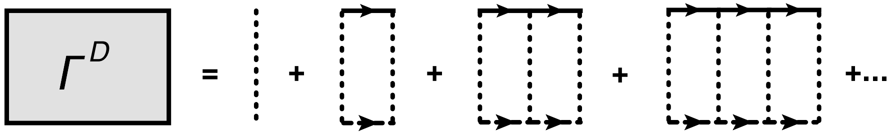
Diffuson

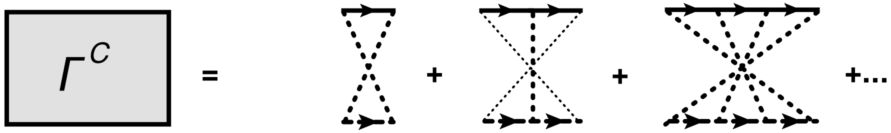
Cooperon



Coherent transport : diagrammatics

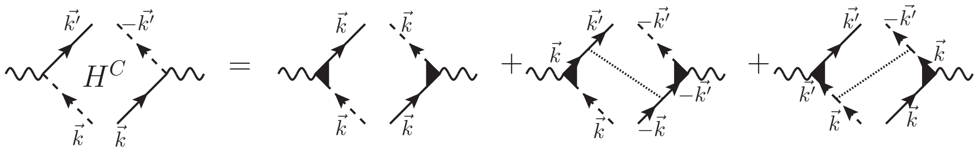
- Interferences effects : 2 diffusive modes





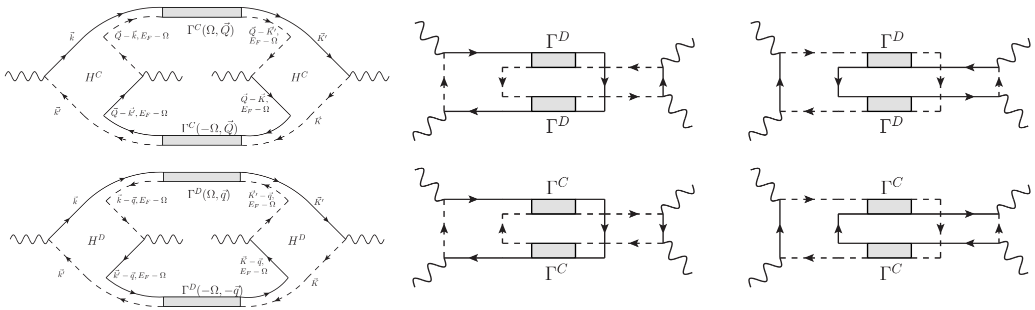
$$\Gamma^C(\vec{Q}) = \gamma \frac{1}{DQ^2\tau_e}\frac{1}{4}\left[Id\otimes Id - \sigma^x\otimes\sigma^x - \sigma^y\otimes\sigma^y - \sigma^z\otimes\sigma^z\right]$$

- Weak anti-localization



$$\langle\delta\sigma\rangle = \frac{e^2}{\pi\hbar}\int_{\vec{Q}}\frac{1}{Q^2}$$

- Conductance fluctuations



$$\langle\delta\sigma^2\rangle = 12\left(\frac{e^2}{h}\right)^2\frac{1}{V}\int_{\vec{q}}\frac{1}{q^4}$$

Same results as non-relativistic electrons
with random spin-orbit coupling !

Anderson problem

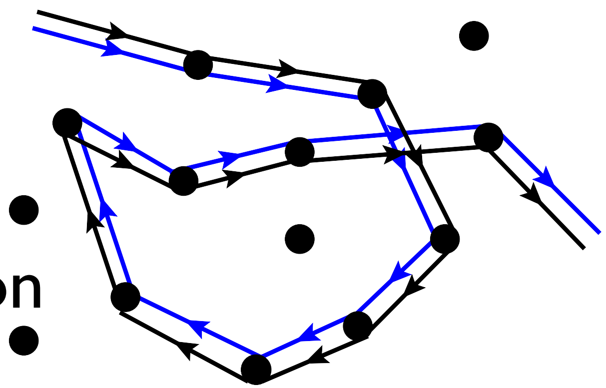
- Coherent metal + weak disorder : Anderson problem
  - Universality classes for transition (strong disorder) : universal metallic properties (weak disorder)
  - Time Reversal Symmetry , $\mathcal{H} = \hbar v_F \left(\vec{k} \times \vec{\sigma}\right) .\hat{z} + V(\vec{r})$
  - $T^2 = -1$

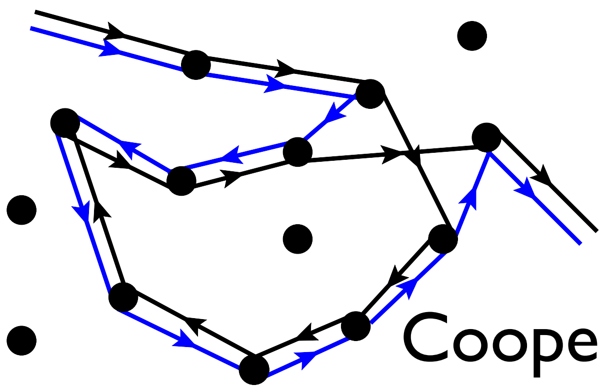
	Symmetry			$d-1$			
	T	P	C	0	1	2	
Wigner - Dyson Classes							
A	0	0	0	0	$\mathbb{Z}$	0	Unitary
AI	1	0	0	0	0	0	Orthogonal
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	Symplectic

- Symplectic class/AII crossover to Unitary/A (mag. field)

2 / 1 diffusive modes

Diffuson



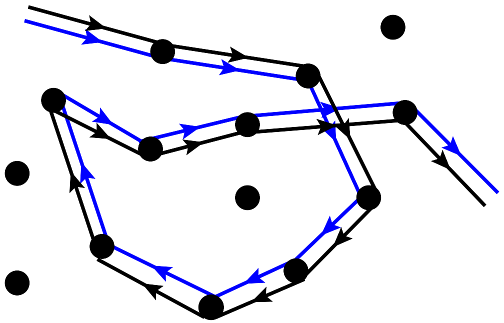


Cooperon

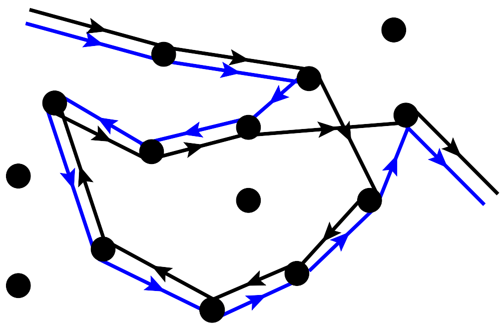
Symplectic and unitary classes results

Symplectic class, TRS

- Diffusive modes



Diffuson



Cooperon

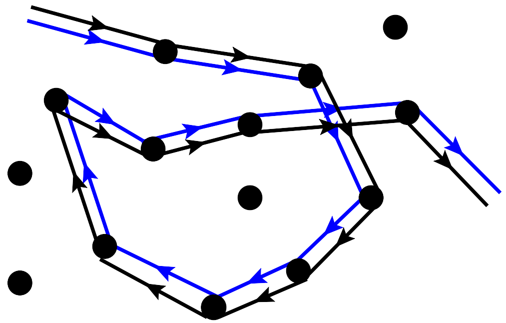
- Weak Anti Localization (WAL)

$$\langle \delta\sigma \rangle = \frac{e^2}{\pi\hbar} \int_{\vec{Q}} \frac{1}{Q^2}$$

- Conductance fluctuations

$$\langle \delta\sigma^2 \rangle = 12 \left(\frac{e^2}{h} \right)^2 \frac{1}{V} \int_{\vec{q}} \frac{1}{q^4}$$

Unitary class



Diffuson

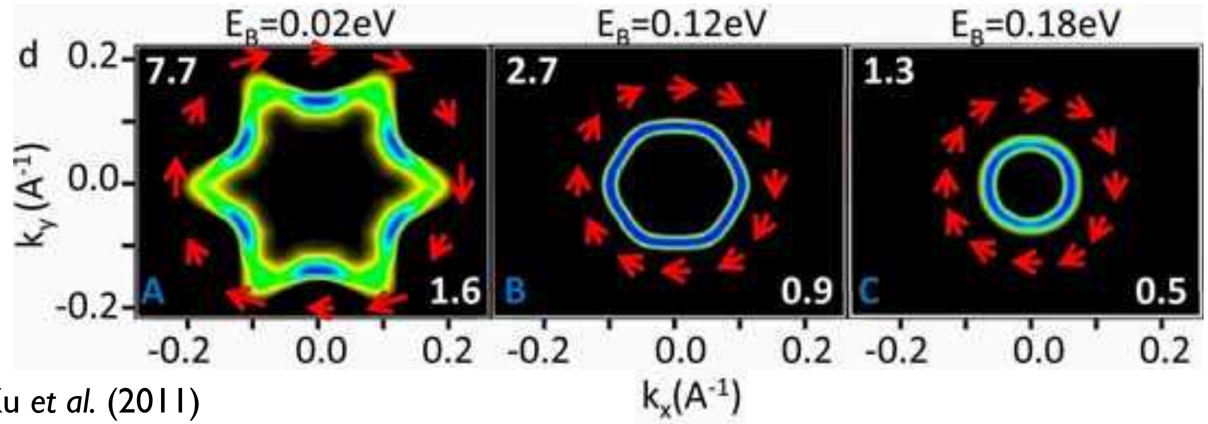
$$\langle \delta\sigma \rangle = 0$$

$$\langle \delta\sigma^2 \rangle = 6 \left(\frac{e^2}{h} \right)^2 \frac{1}{V} \int_{\vec{q}} \frac{1}{q^4}$$

Universal results : specificity of Dirac in the crossovers

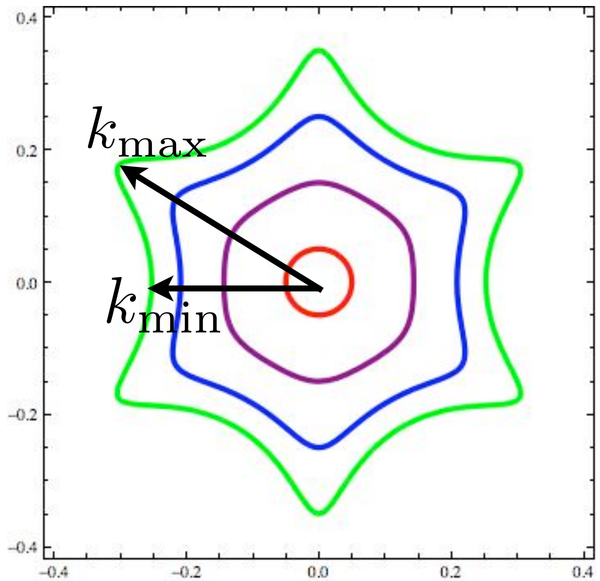
Hexagonal warping

- Fermi surface deformation



S.Y. Xu *et al.* (2011)

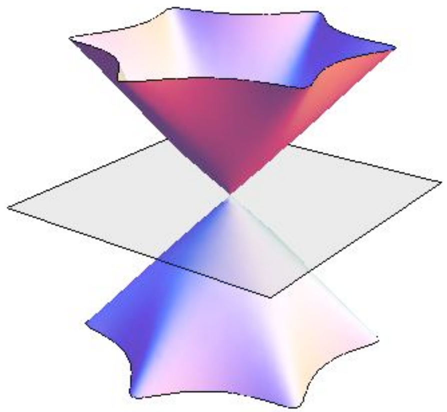
Different energies Fermi surfaces



- Warping hamiltonian

$$\mathcal{H} = \hbar v_F(\vec{\sigma} \times \vec{k}).\hat{z} + \frac{\lambda}{2}(k_+^3 + k_-^3)\sigma^z$$

(L. Fu, 2009)

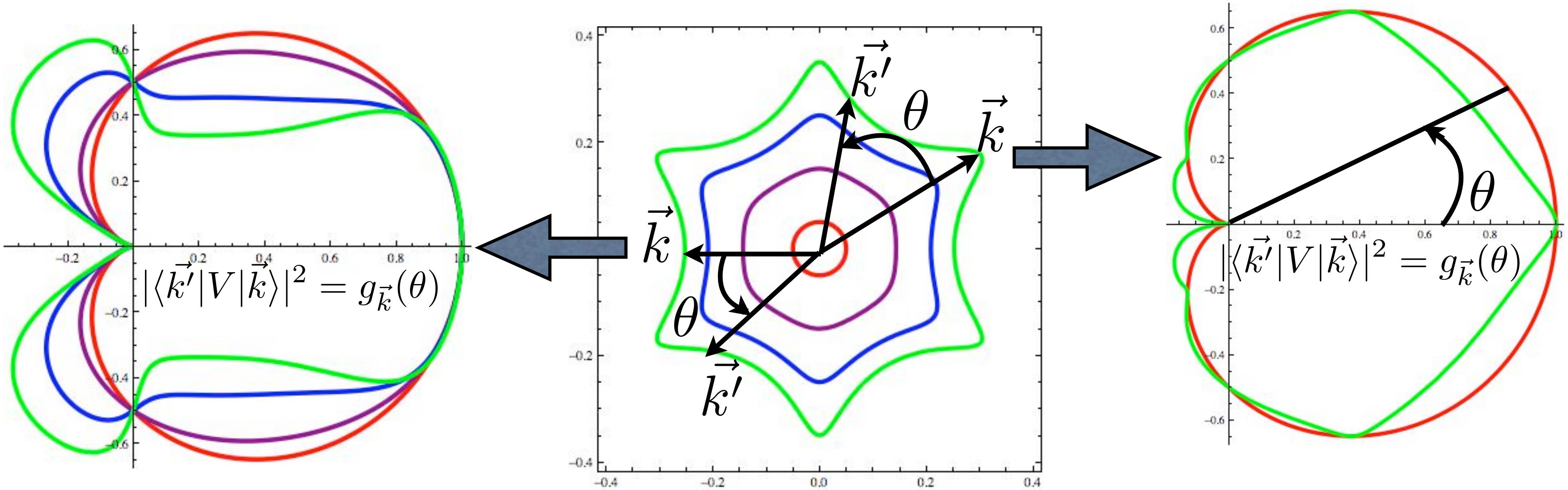


$$b = \frac{\lambda E_F^2}{2(\hbar v_F)^3} = \frac{w(w+w_{\rm max})^2}{2(w_{\rm max}-w)^3} \quad ; \quad w = w_{\rm max}\frac{k_{\rm max}-k_{\rm min}}{k_{\rm max}+k_{\rm min}},$$

Experimentally : $0 \leqslant b \lesssim 0.6$

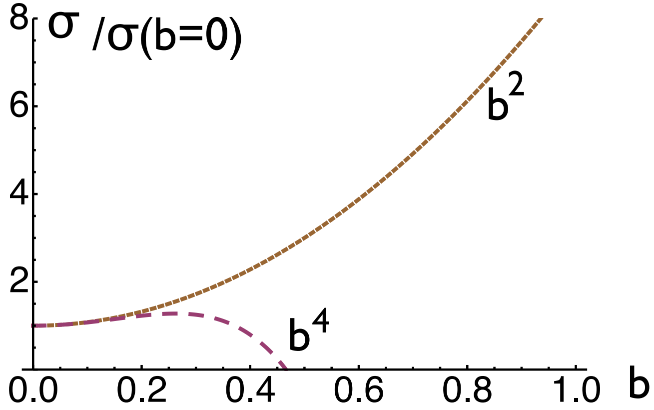
Boltzmann approach

- Density of states : $f(\vec{k})$
- Scattering probability : $|\langle\vec{k'}|V|\vec{k}\rangle|^2 = g_{\vec{k}}(\theta)$ spinor overlap



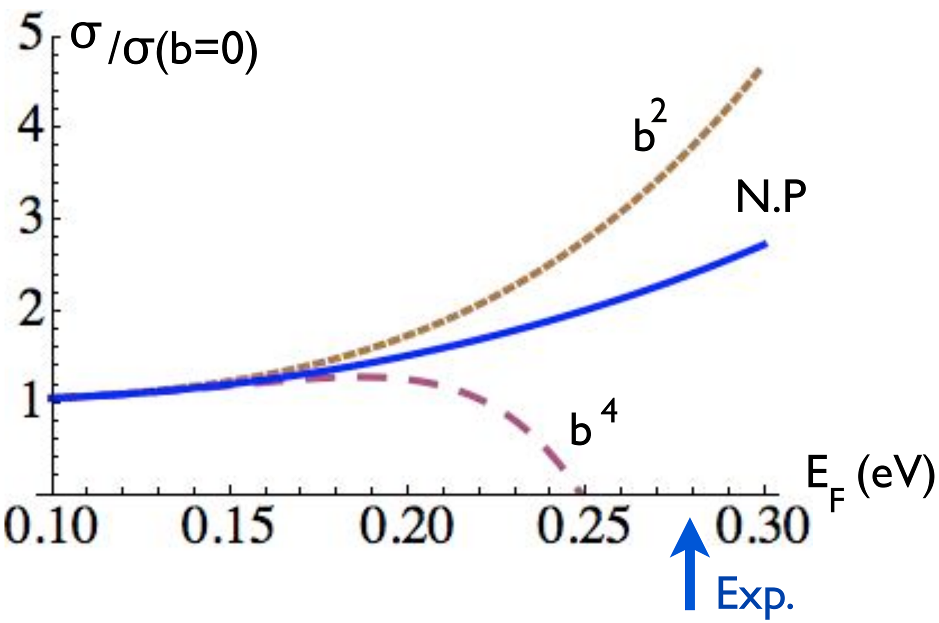
<u>Perturbative result</u>

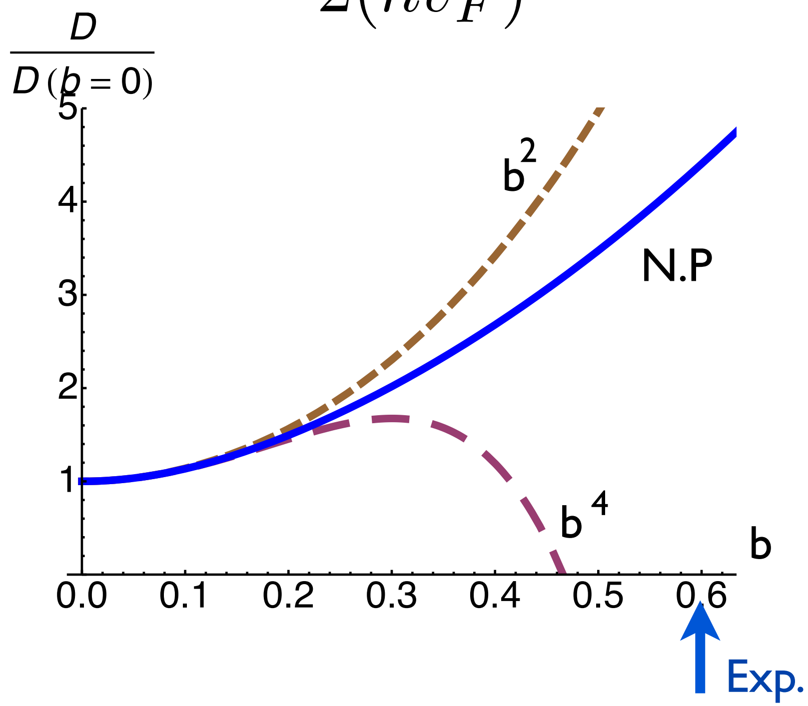
$$\sigma = \frac{e^2}{h}\frac{2\hbar^2 v_F^2}{\gamma}(1 + 8b^2 - 58b^4 + o(b^4))$$



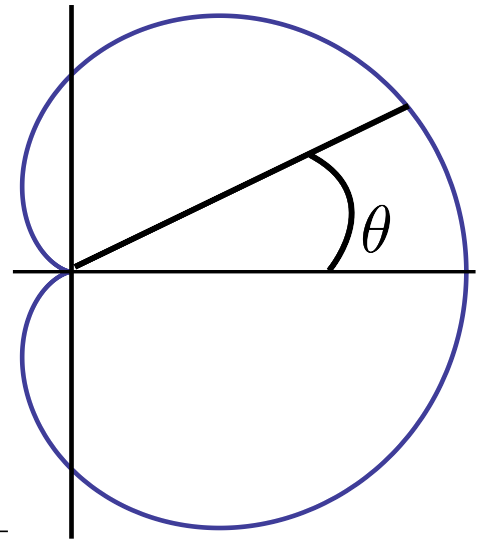
Diagrammatic approach

- Result non perturbative in warping term b
- Correction to Dirac physics
- Possible to probe experimentally $$b = \frac{\lambda E_F^2}{2(\hbar v_F)^3}$$

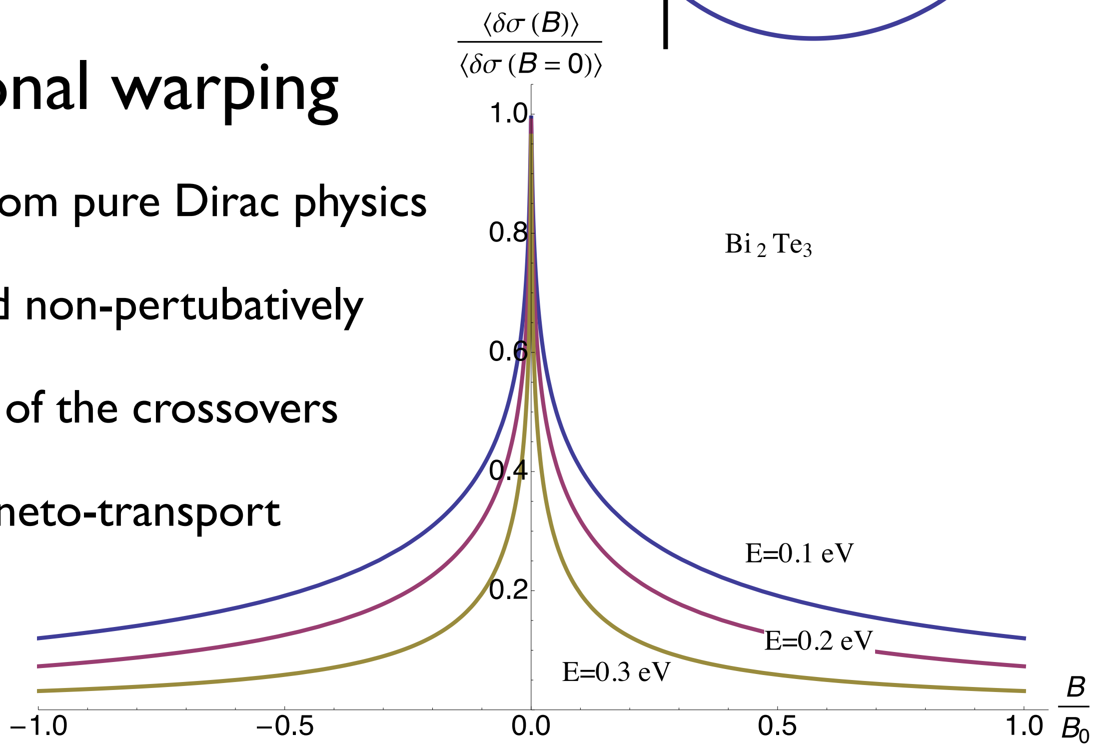




Theory of diffusion of 3DTI surface states



- Dirac physics : anisotropy of the scattering
- Symplectic class, universal result (WAL correction)
- Specificity of the hexagonal warping
  - Departure from pure Dirac physics
  - To be treated non-pertubatively
  - Dependance of the crossovers
  - In-plane magneto-transport



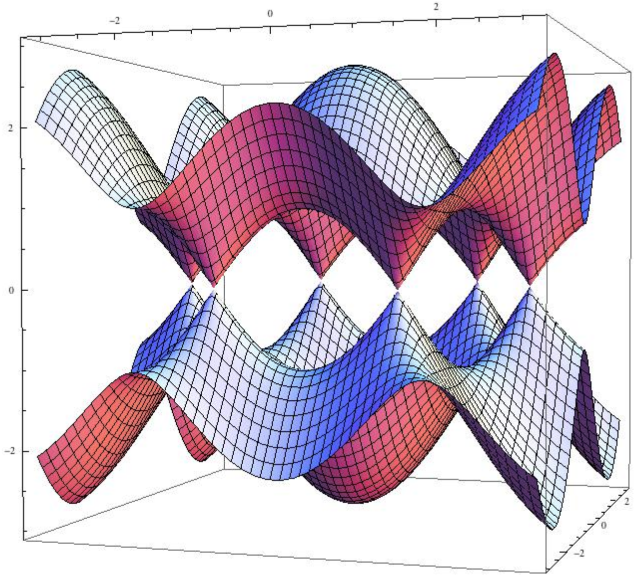
Outline

- Diffusion, regime of weak disorder
- Diffusion of Dirac fermions
  - 3D Strong topological insulators
  - Graphene
- Diffusion of semi-Dirac excitations

Dirac fermions system $\mathcal{H} = \hbar v_f(\vec{\sigma} \times \vec{k}).\hat{z}$

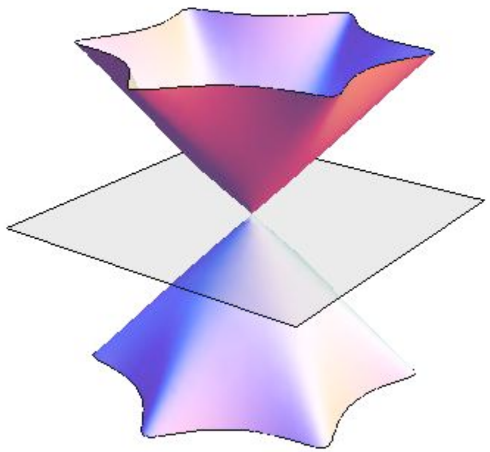
Graphene

- σ : sublattice
- 2 x 2 cones
- TRS : no constraint
- Trigonal warping at high energies



STI surface state

- σ : magnetic spin
- 1 cone (odd)
- TRS : constraint
- Hexagonal warping at high energies



Weak localization in graphene

Valley degeneracy :
possibility of intra- and inter- valley scattering

Intravalley scattering only

- 2 independant Dirac cones
- Absence of backscattering
- Weak anti-localization

With Intervalley scattering

- 2 disorder-coupled Dirac cones
- Possibility of backscattering
- Weak localization

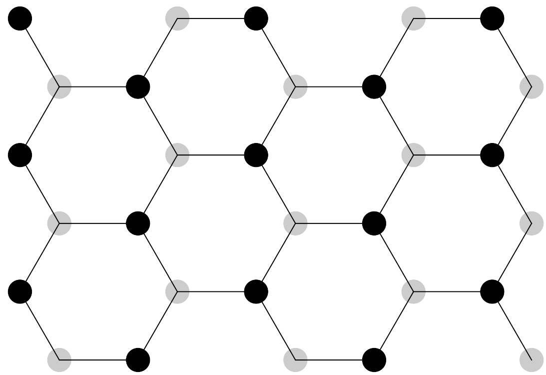
Strong disorder limit :
disorder always opens a gap (insulator) as opposed to 3DSTI (always at least one

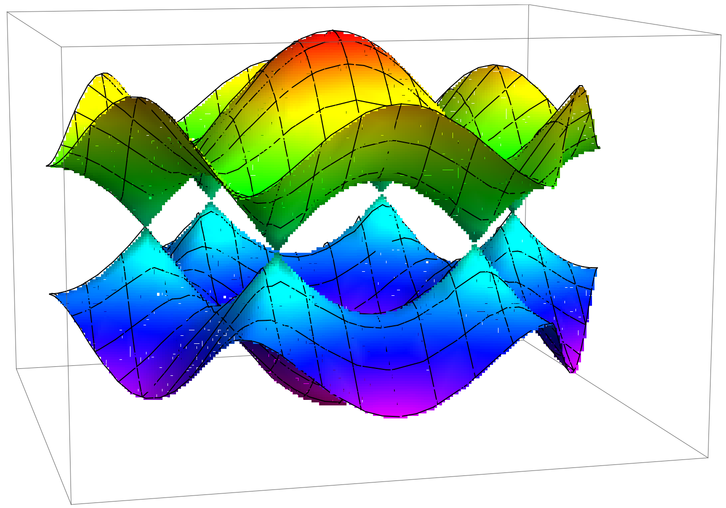
Outline

- Diffusion, regime of weak disorder
- Diffusion of Dirac fermions
    - 3D Strong topological insulators
    - Graphene
- Diffusion of semi-Dirac excitations

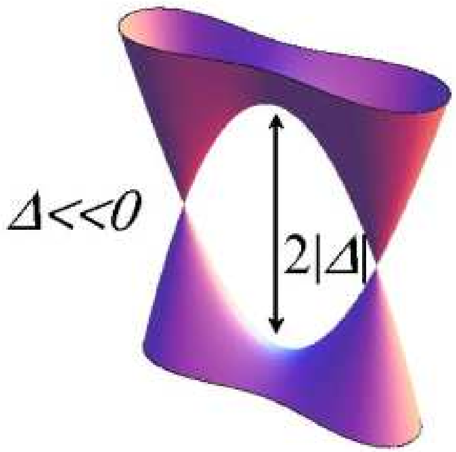
Semi-Dirac excitations

- Hexagonal lattice (graphene)

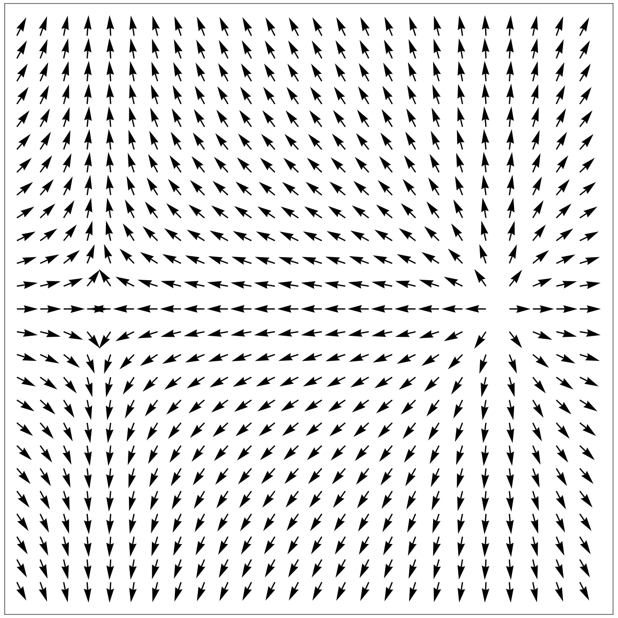




- 2 Dirac fermions, with topologic number



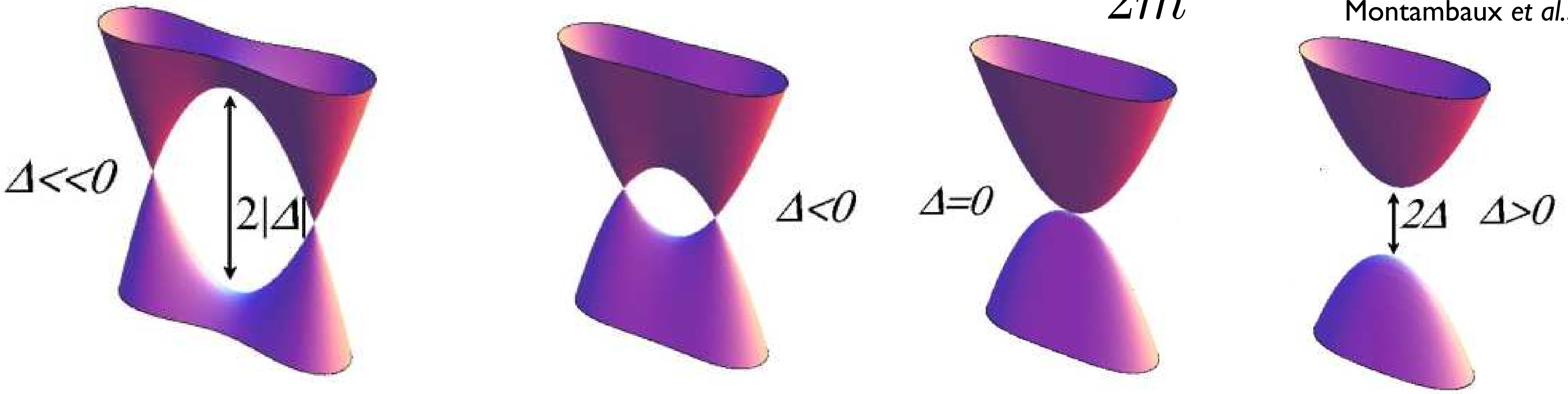
$$\mathcal{H} = \hbar v_F \vec{\sigma}.\vec{q}$$



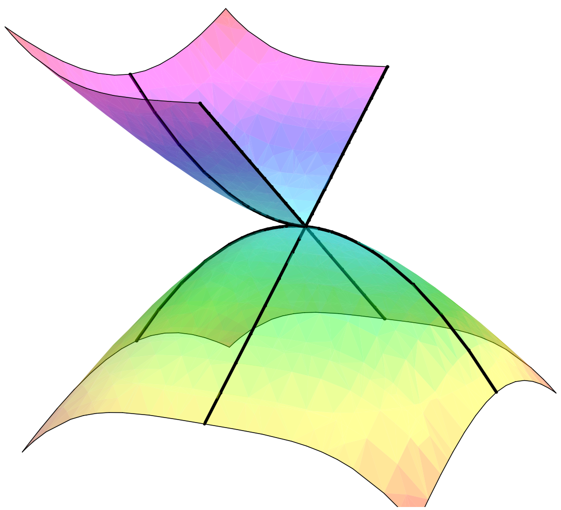
Semi-Dirac excitations

- Merging of the Dirac cones $\mathcal{H} = (\Delta + \frac{\hbar^2 q_x^2}{2m})\sigma^x + \hbar v_F \sigma^y q^y$

Montambaux *et al.*, 2009



- Δ = 0 : Semi-Dirac excitation, $\mathcal{H} = \frac{\hbar^2 q_x^2}{2m}\sigma^x + \hbar v_F \sigma^y q^y$



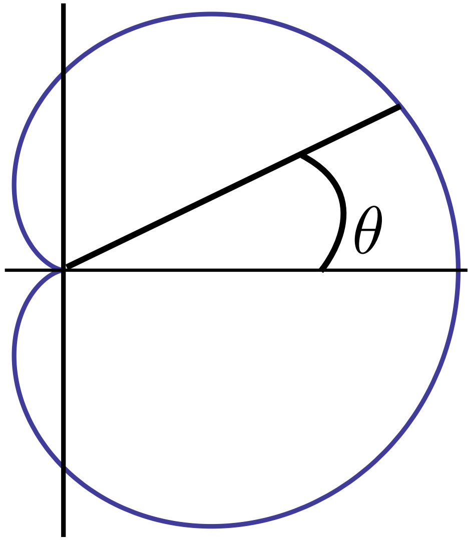
Also predited in VO_2/TiO_2 heterostructures

Pardo and Pickett, 2009

Boltzmann equation

- Spinorial nature : Anisotropy of the scattering

Pure Dirac fermions

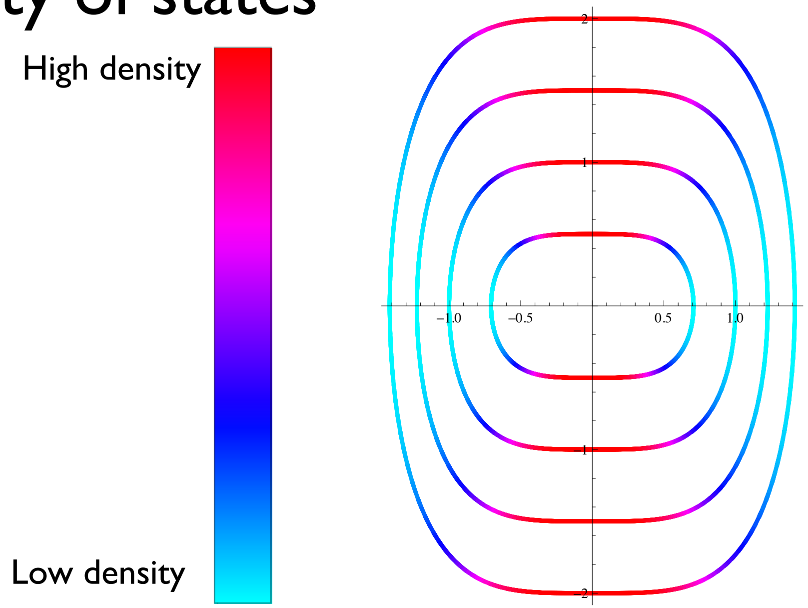


$$|\psi(\vec{k})\rangle = \begin{pmatrix} 1 \\ e^{i\theta_{\vec{k}}} \end{pmatrix}$$

$$|\langle\psi(\vec{k})|\psi(\vec{k'})\rangle|^2 = \frac{1+\cos\theta}{2}$$

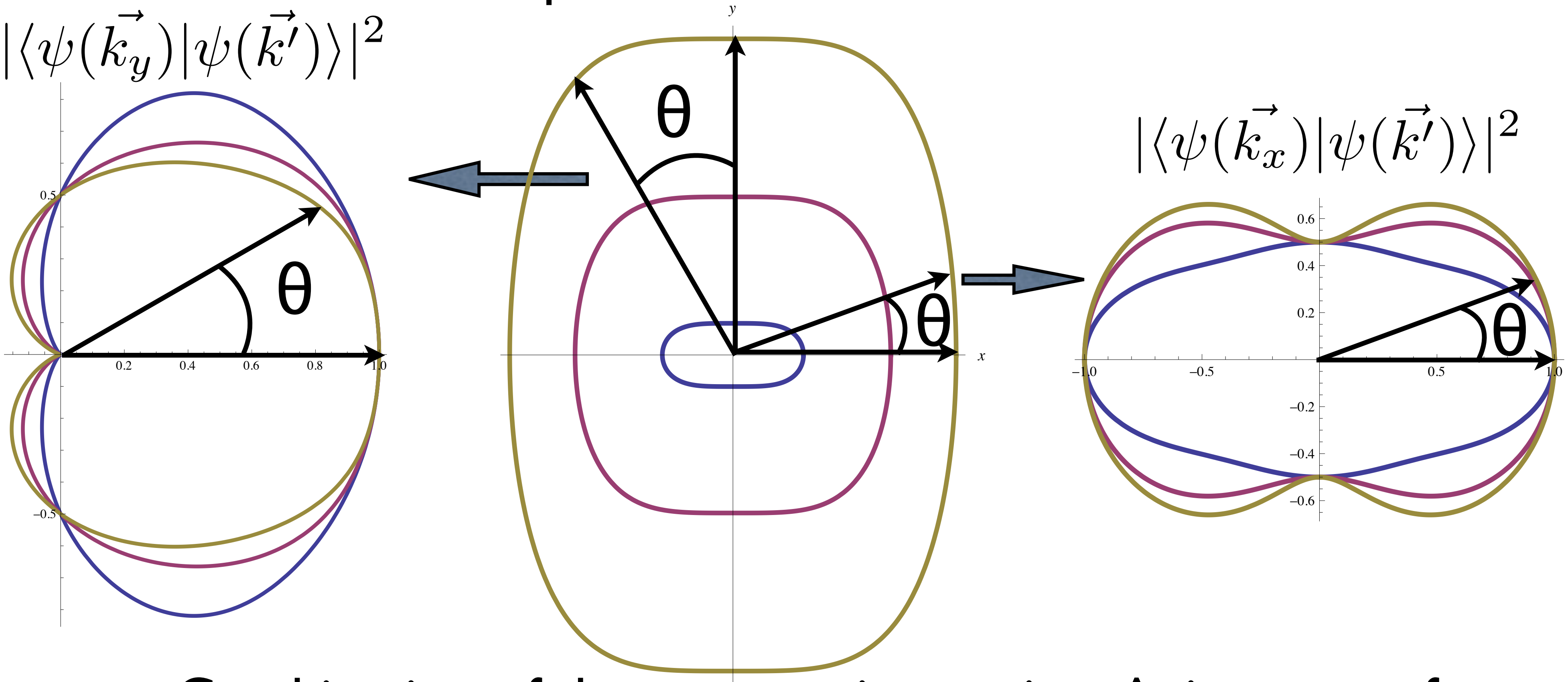
- Anisotropy of the density of states

$$\mathcal{H} = \frac{\hbar^2 q_x^2}{2m}\sigma^x + \hbar v_F \sigma^y q^y$$



Boltzmann equation

- Stronger anisotropy of the scattering for semi-Dirac excitations compared to Dirac fermions



- Combination of these two anisotropies : Anisotropy of the diffusion $D_x \neq D_y$

Diagrammatics

- Direction dependant elastic mean free time

$$-\Im\Sigma = \frac{1}{\tau_e} Id + \frac{\cos\theta}{\tau_e^*}\sigma^x$$

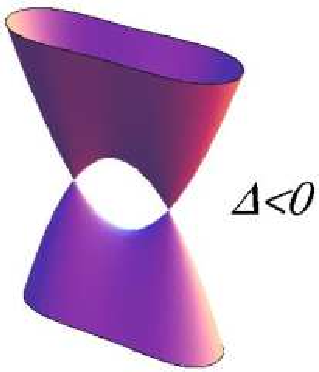
- 2 diffusive modes, 1 diffuson and 1 cooperon
- Drude conductivity tensor

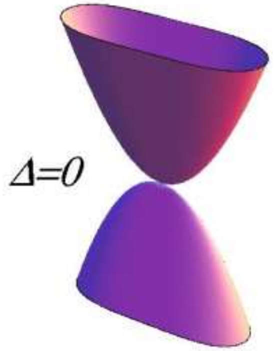
$$\sigma_{xx} = \frac{e^2}{h}\frac{2E\hbar^2}{m\gamma}\frac{2e}{\tilde{a}} \qquad \sigma_{yy} = \frac{e^2}{h}\frac{\hbar^2 v_F^2}{\gamma}\frac{2c}{\tilde{a}} \qquad \sigma_{xy} = \sigma_{yx} = 0$$

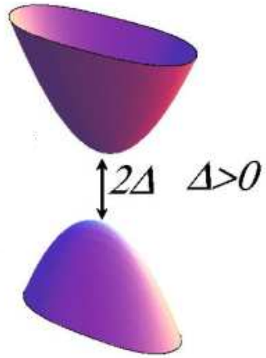
- Weak anti-localization (Quantum interferences)

Topological phase transition

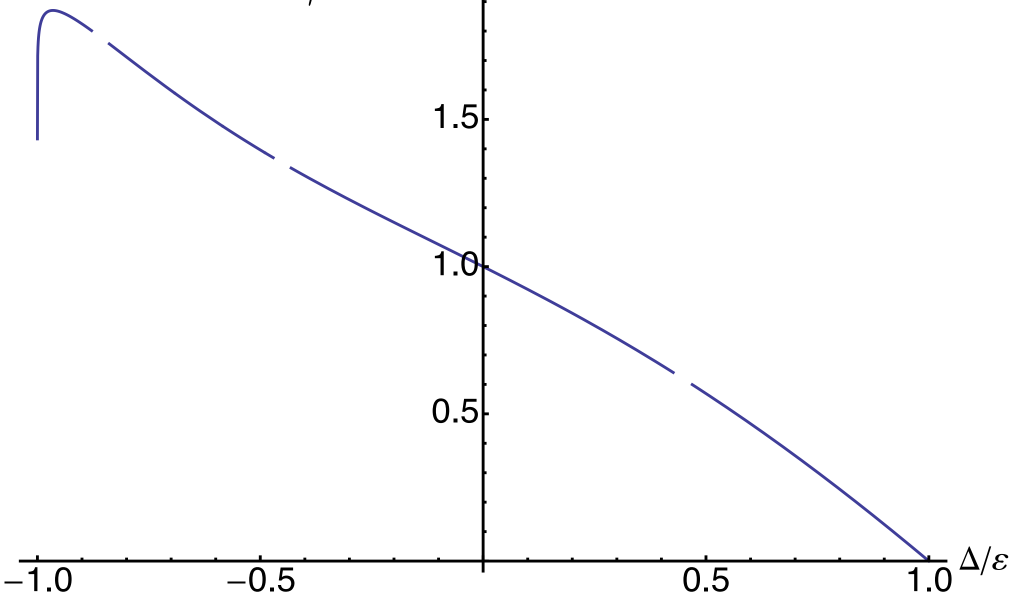
- Dependance in Δ of the conductances



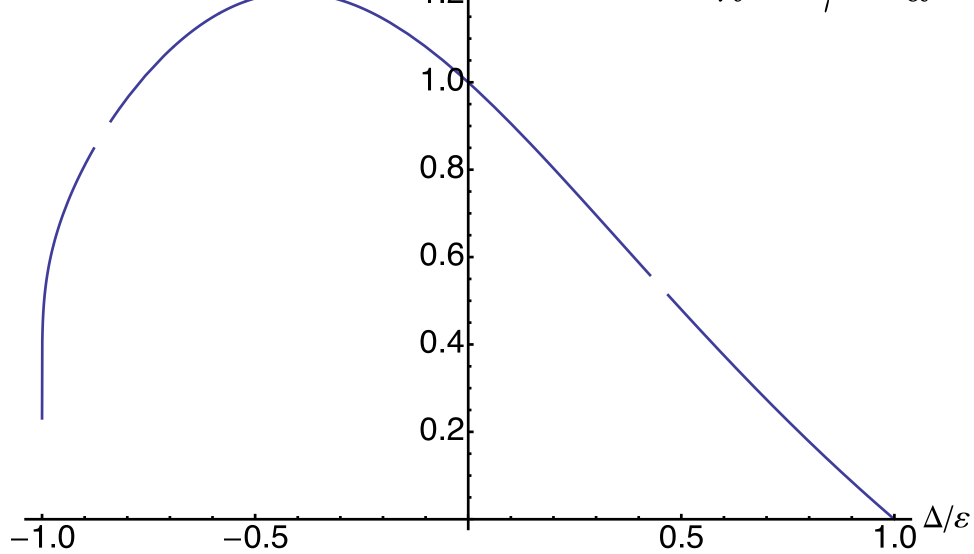




$$\sigma_{xx} = \frac{e^2}{h}\frac{2E\hbar^2}{m\gamma}\frac{2e}{\tilde{a}}$$

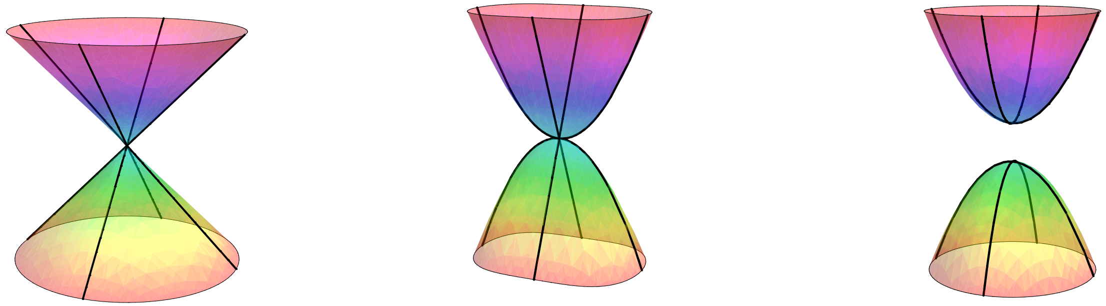


$$\sigma_{yy} = \frac{e^2}{h}\frac{\hbar^2 v_F^2}{\gamma}\frac{2c}{\tilde{a}}$$

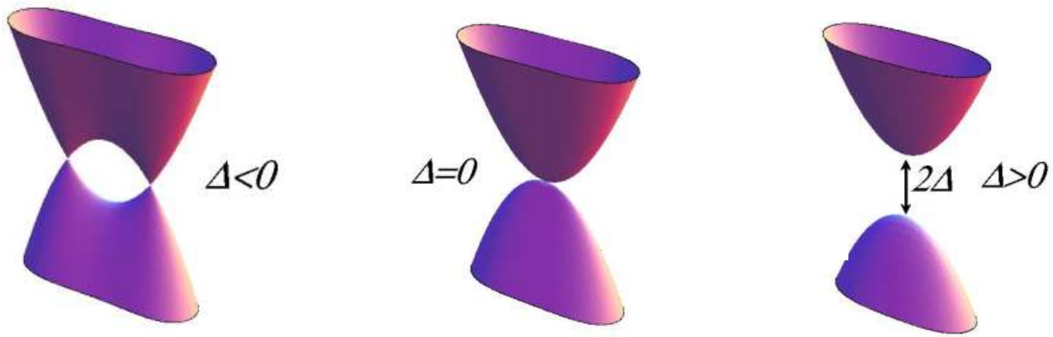


Conclusion

- Significative difference with Dirac or non-relativistic excitations : anisotropic diffusion



- Study of the topological phase transition



- Weak antilocalization (symplectic class)
- Details soon on ArXiv