# Quantum transport in carbon nanotubes and graphenes

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# Outline

- Introduction
  - Suppression of backward scattering
  - Weak-localization and universality class
- Magnetoresistance in graphene by symmetry consideration
  - Time-reversal symmetry in graphene
  - Pseudo-spins in graphene
  - Magnetoresistance

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# Impurity Scattering in Carbon Nanotubes – Absence of Back Scattering –

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The effective potential of an impurity in a $\boldsymbol{k}\cdot\boldsymbol{p}$ scheme is derived in two-dimensional graphite sheet. When the potential range is smaller than the lattice constant, it has an off-diagonal matrix element between K and K′ points comparable to the diagonal element. With the increase of the range, this off-diagonal element decreases rapidly and the diagonal element for envelopes at A and B sites becomes identical. The crossover between these two regimes occurs around the range smaller than the lattice constant. In the latter regime, back scattering between states with $+k$ and $-k$ vanishes identically for the bands crossing the Fermi level in the absence of a magnetic field, leading to an extremely large conductivity. The absence of the back scattering disappears in magnetic fields, giving rise to a huge positive magnetoresistance.

KEYWORDS: graphite, carbon nanotube, fullerene tube, Landau level, magnetoresistance, effective-mass theory

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# Berry's Phase and Absence of Back Scattering in Carbon Nanotubes

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The absence of back scattering in carbon nanotubes is shown to be ascribed to Berry's phase which corresponds to a sign change of the wave function under a spin rotation of a neutrino-like particle in a two-dimensional graphite. Effects of trigonal warping of the bands appearing in a higher order $\boldsymbol{k}\cdot\boldsymbol{p}$ approximation are shown to give rise to a small probability of back scattering.

KEYWORDS: graphite, carbon nanotube, fullerene tube, effective-mass theory, impurity scattering, Berry's phase

# Suppression of backward scattering

- Complete suppression of scattering between two counter-propagating states within a valley

- Destructive interference due to the Berry phase originating from the 2-component spinor

$$\gamma \begin{pmatrix} 0 & \hat{k}_x - \mathrm{i}\hat{k}_y \\ \hat{k}_x + \mathrm{i}\hat{k}_y & 0 \end{pmatrix} \begin{pmatrix} F_A(\boldsymbol{r}) \\ F_B(\boldsymbol{r}) \end{pmatrix} = \varepsilon \begin{pmatrix} F_A(\boldsymbol{r}) \\ F_B(\boldsymbol{r}) \end{pmatrix}$$

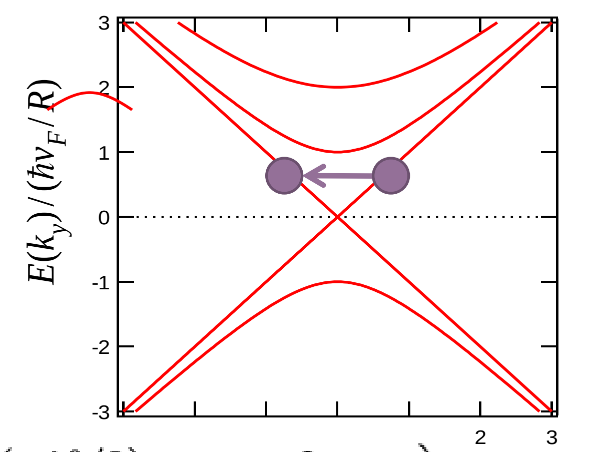
$$\boldsymbol{F}_{s\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{LA}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\, \boldsymbol{F}_{s\boldsymbol{k}},$$

$$\varepsilon_s(\boldsymbol{k}) = s\gamma|\boldsymbol{k}|,$$

$$|s) = \frac{1}{\sqrt{2}} \begin{pmatrix} -\mathrm{i}s \\ 1 \end{pmatrix}$$

$$\boldsymbol{F}_{s\boldsymbol{k}} = \exp[\mathrm{i}\phi_s(\boldsymbol{k})]\, R^{-1}[\theta(\boldsymbol{k})]\, |s),$$

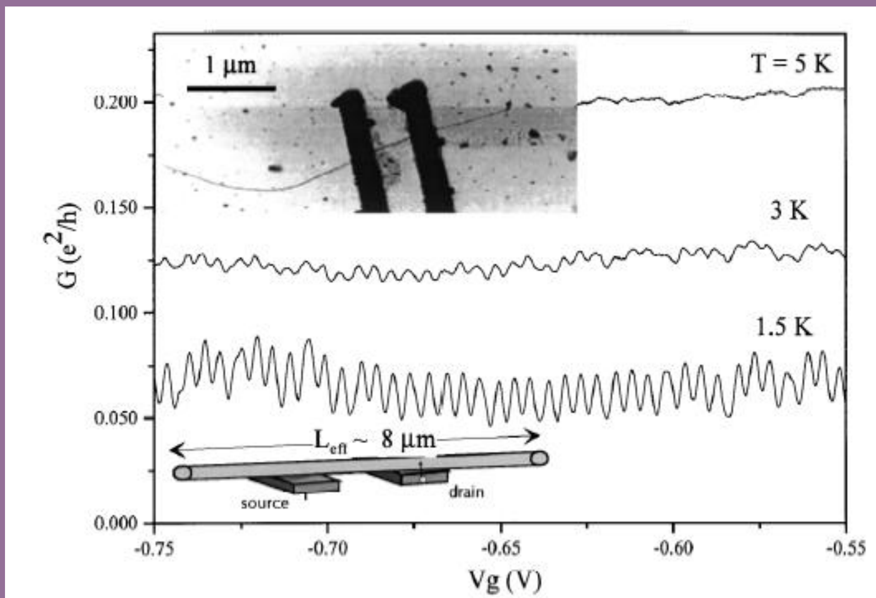
$$R(\theta) = \exp\left(\mathrm{i}\frac{\theta}{2}\sigma_z\right) = \begin{pmatrix} \exp(+\mathrm{i}\theta/2) & 0 \\ 0 & \exp(-\mathrm{i}\theta/2) \end{pmatrix}$$



# Experimental realization

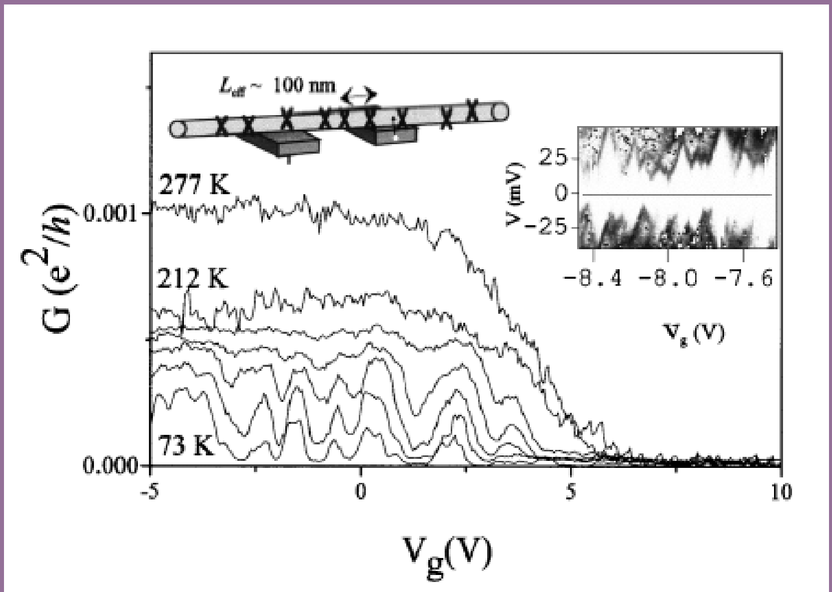
- Conductance measurement : [McEuen et al. PRL(1999)]

Metallic nanotube




Regular coulomb oscillation
→ Leff ~8μm

Doped semiconducting nanotube



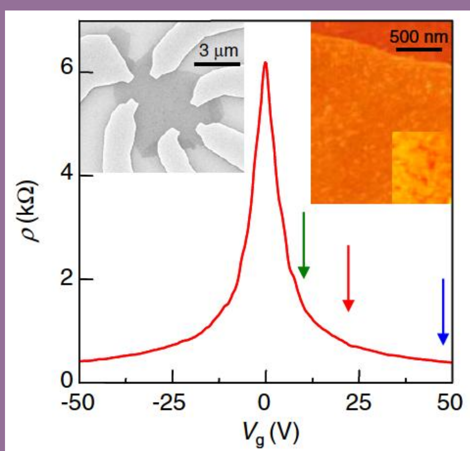

Irregular coulomb oscillation
→ Leff ~100nm

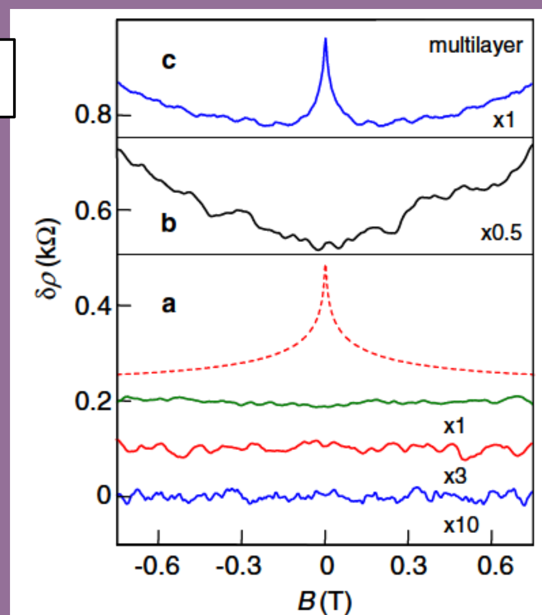
# Magnetoresistance in graphene

- Non-universal behavior (Sample dependent?)

Morozov et al. PRL(2006)

Graphene on $SiO_2$

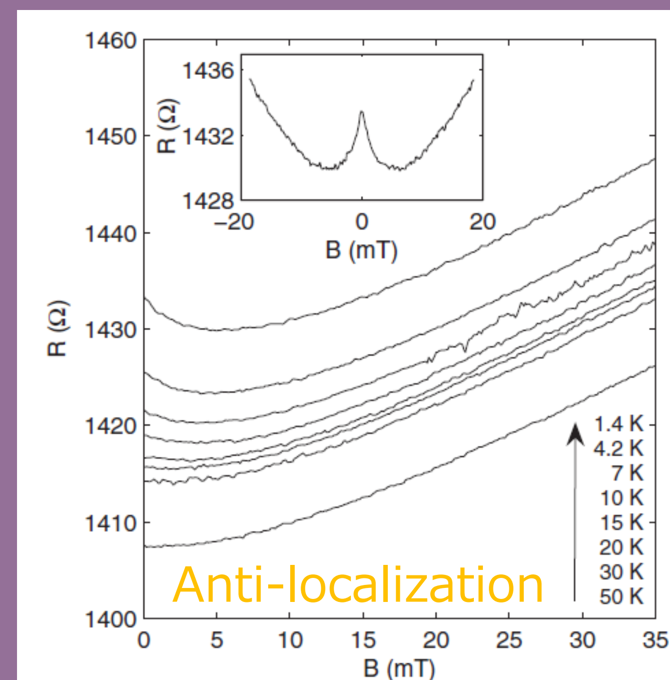



Suppression of WL correction

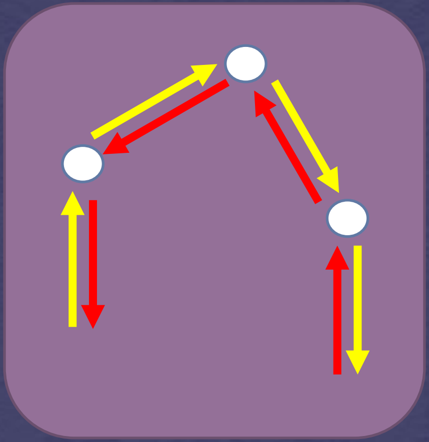
Wu et al. PRL(2007)

Epitaxial graphene



# Weak localization (WL)

- Scattering Probability



Classical : $P_C = | A |^2 + | B |^2$

Quantum : $P_Q = | A + B |^2$
$= | A |^2 + | B |^2 + 2 \mathrm{Re}[ A B^* ]$

Time-reversal symmetry → $A = B$ → $P_Q = 2P_C$

Constructive interference enhances the scattering.
→ Negative quantum correction to conductivity
= Weak localization (WL) correction

# Universality class for localization

- Classification by fundamental symmetry :

  Time-reversal symmetry (TRS)

  Spin-rotational symmetry (SRS)

| | TRS | SRS | WL correction |
|---|---|---|---|
| Orthogonal | Yes | Yes | Negative |
| Unitary | No | Yes or No | 0 |
| Symplectic | Yes | No | Positive |

Positive WL correction for the system with spin-orbit interaction

→ Anti (weak) localization

# Magnetoresistance (MR)

- Classical resistivity is independent of magnetic field.
- Magnetic field breaks TRS.
  → WL correction vanishes! (Crossover)

Orthogonal class → Unitary class (Negative MR)

Symplectic class → Unitary class (Positive MR)

# How about graphene and nanotube?

- No symmetry breaking term for TRS and SRS.
  → Orthogonal class
- Suppression of backward scattering
  → Symplectic class
- No (or non-universal) magnetoresistance
  → Unitary class

# Time-reversal symmetry

- Time-reversal operation : $\mathrm{T} = \mathrm{UC}$

(U : Unitary matrix, C : complex conjugation)

Wave function : $\Psi^R = \mathrm{T}\Psi = \mathrm{U}\Psi^*$

Operator : $X^R = \mathrm{T}X^\dagger\mathrm{T}^\dagger = \mathrm{U}X^T\mathrm{U}^\dagger$

Schrödinger eq.: $i\frac{\partial}{\partial t}\Psi = H\Psi \Rightarrow i\frac{\partial}{\partial(-t)}\Psi^R = H^R\Psi^R$

Matrix element : $\langle\phi|\varphi\rangle = \langle\varphi^R|\phi^R\rangle$ $\langle\phi|X|\varphi\rangle = \langle\varphi^R|X^R|\phi^R\rangle$

- Key property : $\mathrm{T}^2 = +1$ or $\mathrm{T}^2 = -1$

# Amplitude for backward scattering

- Backward scattering : $|\alpha\rangle \Leftrightarrow |\mathrm{T}\alpha\rangle = |\alpha^R\rangle$
- Scattering amplitude : $A = \langle \alpha^R | V | \beta \rangle \langle \beta | V | \alpha \rangle$

  $B = \langle \alpha^R | V | \beta^R \rangle \langle \beta^R | V | \alpha \rangle$

- Time-reversal symmetry:

$$A = \langle \beta^R | V^R | (\alpha^R)^R \rangle \langle \alpha^R | V^R | \beta^R \rangle = \langle \alpha^R | V | \beta^R \rangle \langle \beta^R | V | \mathrm{T}^2 \alpha \rangle = \pm B$$

- Interference between *A* and *B* :

  $\mathrm{T}^2 = +1$ → Constructive → Weak localization

  $\mathrm{T}^2 = -1$ → Destructive → Anti-localization

# Universality class for localization

- Classification by time-reversal symmetry :

| | TRS | WL correction |
|---|---|---|
| Orthogonal | $T^2=+1$ | Negative |
| Unitary | No | 0 |
| Symplectic | $T^2=-1$ | Positive |

Random matrix theory
[Dyson JMP (1962)]

Find the operator T satisfying the following relation:

$$H^R = \mathrm{T} H^\dagger \mathrm{T}^\dagger = \mathrm{U} H^\mathrm{T} \mathrm{U}^\dagger = H$$

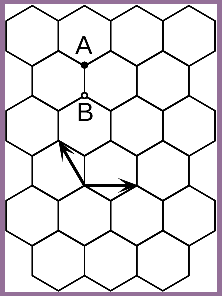
( T=UC, *H*: Effective Hamiltonian )

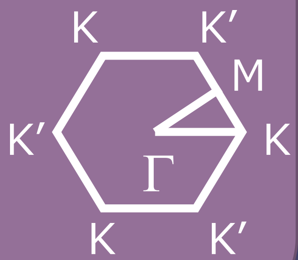
# Effective-mass equations

- 4-component massless Dirac equation

$$\gamma\begin{bmatrix} 0 & k_x - ik_y & 0 & 0 \\ k_x + ik_y & 0 & 0 & 0 \\ 0 & 0 & 0 & k_x + ik_y \\ 0 & 0 & k_x - ik_y & 0 \end{bmatrix}\begin{bmatrix} F_A^K \\ F_B^K \\ F_A^{K'} \\ F_B^{K'} \end{bmatrix} = \varepsilon\begin{bmatrix} F_A^K \\ F_B^K \\ F_A^{K'} \\ F_B^{K'} \end{bmatrix}$$

Honeycomb lattice




Brillouin zone

- Representation by Pauli matrices

$$\mathrm{H}_0 = \gamma\begin{bmatrix} k_x\sigma_x + k_y\sigma_y & \mathrm{O} \\ \mathrm{O} & k_x\sigma_x - k_y\sigma_y \end{bmatrix}$$

$$= \gamma\left[k_x\left(\sigma_x \otimes 1_2\right) + k_y\left(\sigma_y \otimes \tau_z\right)\right]$$

(A & B) → $\begin{pmatrix}\sigma_x & \sigma_y & \sigma_z\end{pmatrix}$

(K & K′) → $\begin{pmatrix}\tau_x & \tau_y & \tau_z\end{pmatrix}$

# Candidates for time-reversal operation

- Normal time-reversal operation

$$\mathrm{T} = (\sigma_z \otimes \tau_x)\mathrm{C} \qquad \mathrm{T}^2 = \sigma_z^2 \otimes \tau_x^2 = 1_2 \otimes 1_2 = 1$$

- Special time-reversal operation

$$\mathrm{S}_x = -i(\sigma_y \otimes 1_2)\mathrm{C} \qquad \mathrm{S}_y = -(\sigma_y \otimes \tau_z)\mathrm{C} \qquad \mathrm{S}_z = i(\sigma_z \otimes \tau_y)\mathrm{C}$$

$$\mathrm{S}_x^2 = \mathrm{S}_y^2 = \mathrm{S}_z^2 = -1$$

- Conserved pseudo-spin : $[H_0, J_n] = 0$

$$J_x = \sigma_x \otimes \tau_x \qquad J_y = \sigma_x \otimes \tau_y \qquad J_z = 1_2 \otimes \tau_z \qquad \mathrm{S}_n = J_n \mathrm{T}$$

# Pseudo-spin representation

- Hamiltonian

$$H_0 = \gamma\left(k_x L_x + k_y L_y\right) = \gamma\left(\vec{k}\cdot\vec{L}\right)$$

$$\vec{L} = \left(\sigma_x \otimes 1_2 \quad \sigma_y \otimes \tau_z \quad \sigma_z \otimes \tau_z\right)$$

$$\vec{k} = \left(k_x \quad k_y \quad 0\right)$$

- Conserved pseudo-spin

$$\vec{J} = \left(\sigma_x \otimes \tau_x \quad \sigma_x \otimes \tau_y \quad 1_2 \otimes \tau_z\right)$$

$$\vec{L} \approx \vec{J} \approx \vec{\sigma}$$

$$\left[H_0, J_n\right] = \left[L_m, J_n\right] = 0$$

- Time-reversal operation

$$\mathrm{T} = \left(iL_y\right)\left(iJ_y\right)\mathrm{C}$$

- Special time-reversal operation:

$$\vec{\mathrm{S}} = \left(J_z \quad -i \quad -J_x\right)\left(\text{-i}L_y\mathrm{C}\right) \approx \text{-i}L_y\mathrm{C}$$

# Impurity potential

- Impurity potential : $u(\mathbf{r}-\mathbf{R}) = \frac{\sqrt{3}}{4\pi\lambda^2} V_0 \exp\left[-\frac{|\mathbf{r}-\mathbf{R}|^2}{(\lambda a)^2}\right]$
- Potential in the effective-mass equation

$$U(\vec{r}) = \begin{bmatrix} u_A(\vec{r}) & 0 & e^{i\phi_A} u'_A(\vec{r}) & 0 \\ 0 & u_B(\vec{r}) & 0 & e^{i\phi_B} u'_B(\vec{r}) \\ e^{-i\phi_A} u'_A(\vec{r}) & 0 & u_A(\vec{r}) & 0 \\ 0 & e^{-i\phi_B} u'_B(\vec{r}) & 0 & u_B(\vec{r}) \end{bmatrix}$$

- Diagonal elements : $u_\alpha(\vec{r}) \approx u(\vec{r}_\alpha - \vec{R}_0)$
- Off-diagonal elements :

$u'_\alpha(\vec{r}) \approx u(\vec{r}_\alpha - \vec{R}_0) \exp\left[i(\vec{K}-\vec{K}')\cdot\vec{r}_\alpha\right]$ → Rapidly oscillating phase

# Long-range impurity

- Off-diagonal terms are negligible when the potential range is larger than the lattice constant.

$$U_L(\vec{r}) = \sum_n u_n^L \delta(\vec{r} - \vec{R}_n) \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \sum_n u_n^L \delta(\vec{r} - \vec{R}_n)(1_2 \otimes 1_2)$$

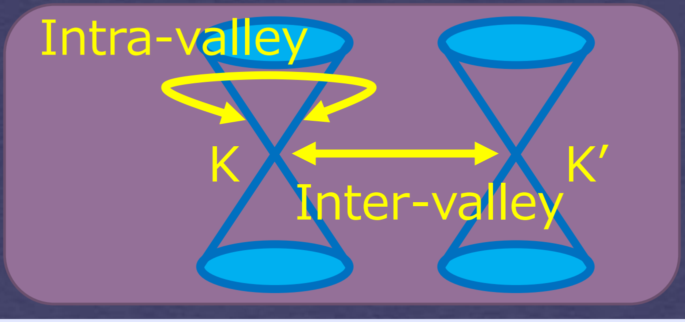
- Hamiltonian does not contain pseudo-spin $J$.
  → We can omit this pseudo spin.
- Special TRS : $\mathrm{S} = \text{-i}L_y\mathrm{C}$ $\mathrm{S}^2 = (\text{-i}L_y)^2 = -1$

→ Symplectic symmetry is realized! → Antilocalization

# Short-range impurity

- Extremely short potential range (localized at A sites)

$$U_S^A(\vec{r}) = \sum_n u_n^A \delta(\vec{r} - \vec{R}_n) \begin{bmatrix} 1 & 0 & e^{i\phi_n^A} & 0 \\ 0 & 0 & 0 & 0 \\ e^{-i\phi_n^A} & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$




$$= \sum_n u_n^A \delta(\vec{r} - \vec{R}_n) \frac{1}{2} \left[ 1 + L_z J_z + \cos\phi_n^A (L_x J_x + L_y J_y) + \sin\phi_n^A (L_x J_y - L_y J_x) \right]$$

- Pseudo-spin J is not conserved.
- No special TRS : $\mathrm{T} = (iL_y)(iJ_y)\mathrm{C}$ $\quad \mathrm{T}^2 = (iL_y)^2 (iJ_y)^2 = 1$

→ Orthogonal class → Weak localization

# Symmetry crossover

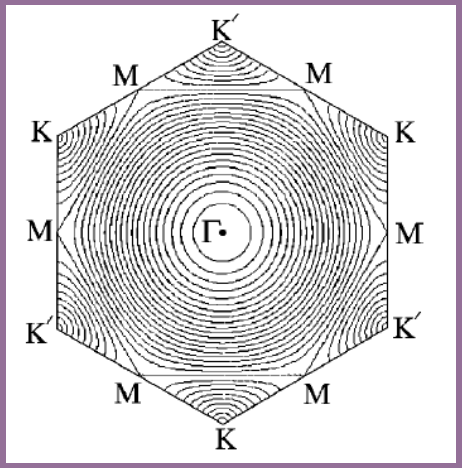
- Symmetry at zero temperature = Orthogonal
- Crossover between symplectic and orthogonal

  $L_S$ : mean free path due to short-range potential (SRP)
  $L_L$ : mean free path due to long-range potential (LRP)
  $L_T$ : phase coherence length
- Assumption : $L_S >> L_L$
- Low temperature limit : $L_T >> L_S$
  → SRP is dominant. → Orthogonal class
- Intermediate temperature : $L_S >> L_T >> L_T$
  → LRP is dominant. → Symplectic class

[ Suzuura, Ando PRL(2002)]

# Magnetoresistance in graphene

- No symmetry-breaking term
  → Positive or Negative MR
  Temperature dependent crossover
  [ Wu et al. PRL(2007)]
- Terms giving inter-valley scattering
  → Negative MR
  Edges, Point defects, etc.




Trigonal warping:
[Saito et al. PRB(2000)]

- Trigonal-warping
  Break special TRS, but give no inter-valley scattering
  → Suppression of MR (No anti-localization)
  [Morozov et al. PRL(2006)] [McCann et al. PRL(2006)]

# Bi-layer graphene

- Effective Hamiltonian :

$$H_0 = \frac{\hbar^2}{2m}\begin{bmatrix} 0 & (k_x - ik_y)^2 \\ (k_x + ik_y)^2 & 0 \end{bmatrix}$$

[ McCann, Falko PRL(2006)]

[ Koshino, Ando PRB(2006)]

- (Special) time-reversal operation : $S = \sigma_x C$

$S^2 = (\sigma_x)^2 = 1$ → Orthogonal (Pseudo-spin conserved!)

- Trigonal warping breaks the special TRS.
→ Suppression of MR (disappearance of WL)

[Kechedzhi et al. PRL(2007)]

# Summary

- Massless Dirac particle + Long-range potential
  → Symplectic class
- + Weak short-range potential
  → Temperature dependent crossover
  between symplectic and orthogonal classes
- +Trigonal warping
  → Unitary class
  → Suppress the magnetoresistance
- Short-range potential breaks all the stories above.