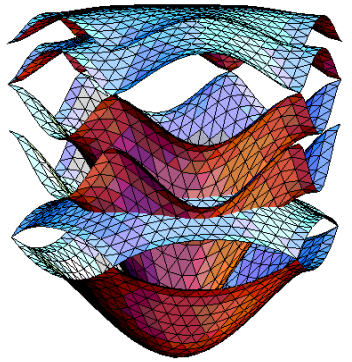
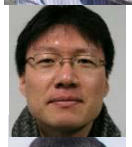
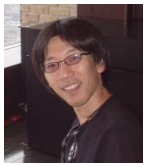
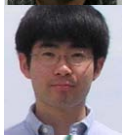
東北大学
TOHOKU UNIVERSITY



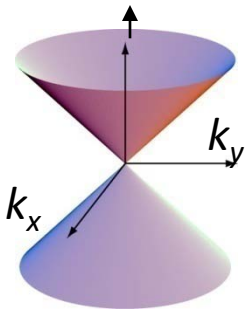
The 1st GCOE international symposium
"Weaving Science Web beyond Particle-Matter Hierarchy"
2009.3.5-7, Sendai, Japan



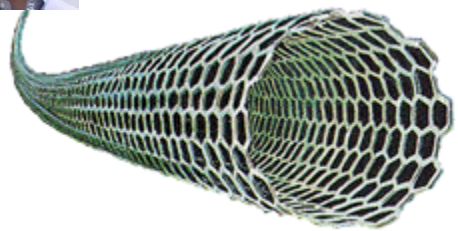
Graphene and Carbon Nanotubes

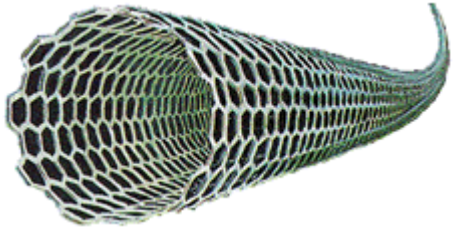
R. Saito
Tohoku University
http://flex.phys.tohoku.ac.jp





K. Nomura

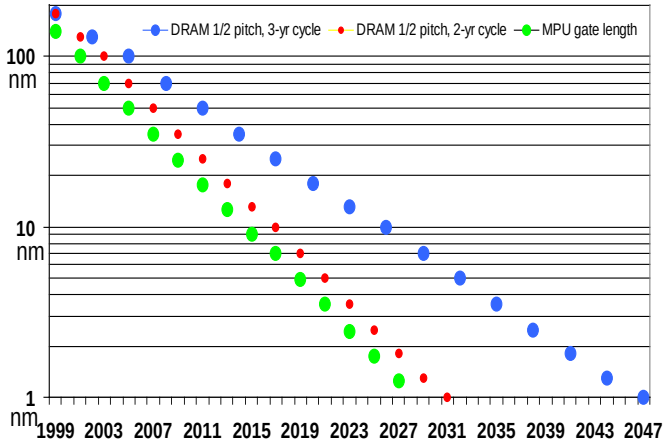




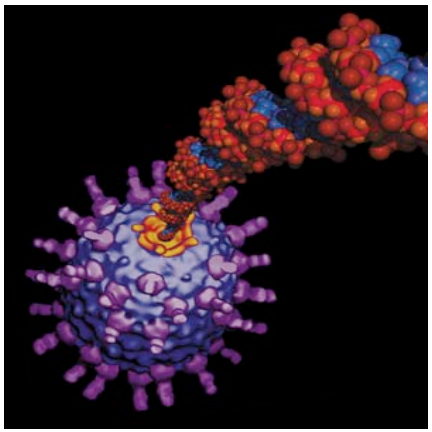
Why do we need nano-materials?

Carbon Nanotubes and Graphene are Important For Motivating the Nanoworld

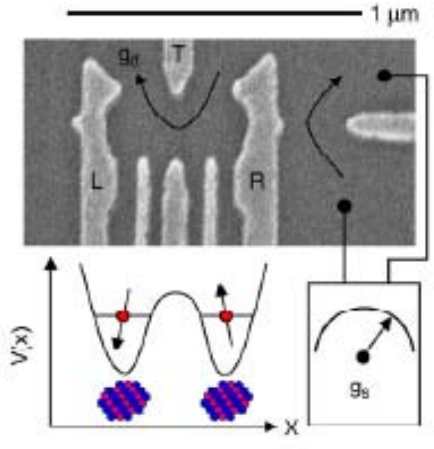
- The Shrinking of Electronics and Moore's Law
- Rapid advances in molecular Biology at the nanoscale
- Evolution of Materials Chemistry from a molecule to a quantum dot



Moore's Law

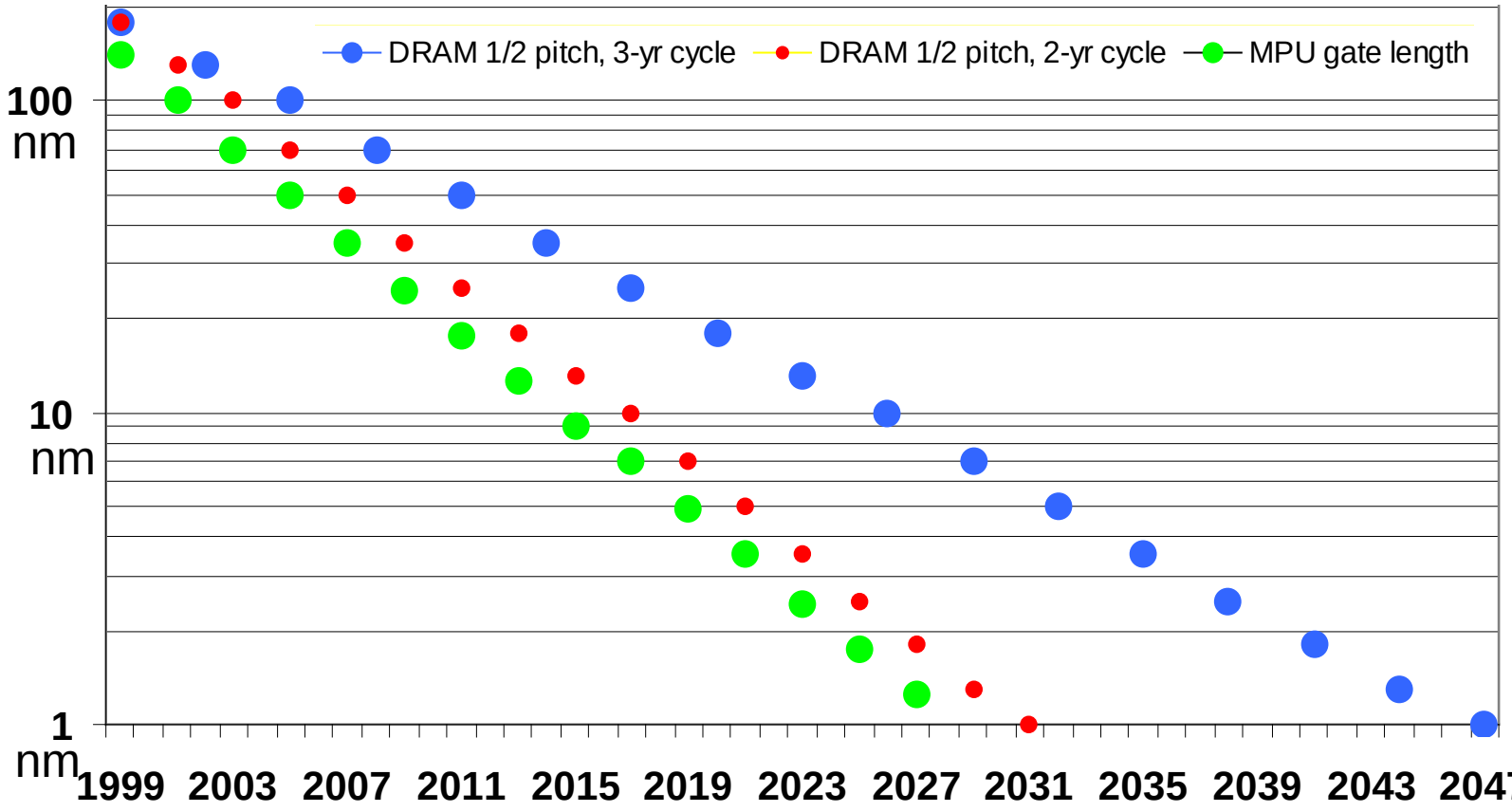


Biology at the nanoscale



Molecule quantum dot

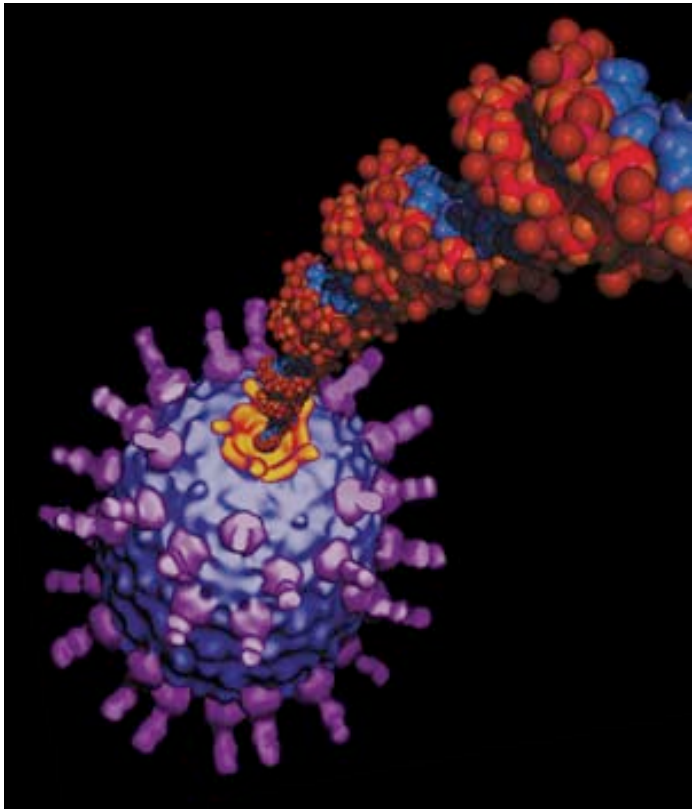
Moore's Law For Semiconductor Electronics
Soon, All Microchips Will Be nanoscale Devices



Semiconductor devices were approaching the nano scale when nanotubes had their official birthday.

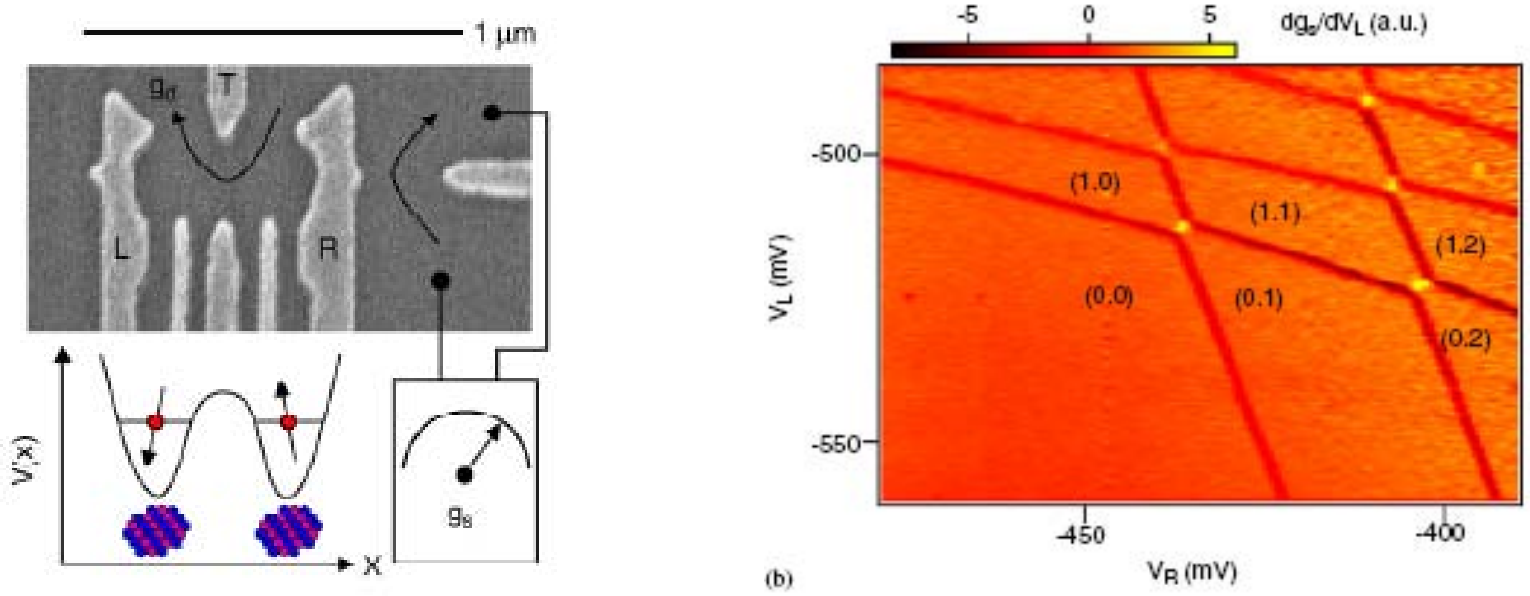
Biological Building Blocks in the Nanoworld

Artist's conception of a DNA strand being packed inside a virus capsid by a molecular motor. The rotary motor of the virus exerts a force of 60 pN to compress the DNA to 6000 times its normal volume. The internal pressure thus generated is later used by the virus to launch this DNA into a cell.



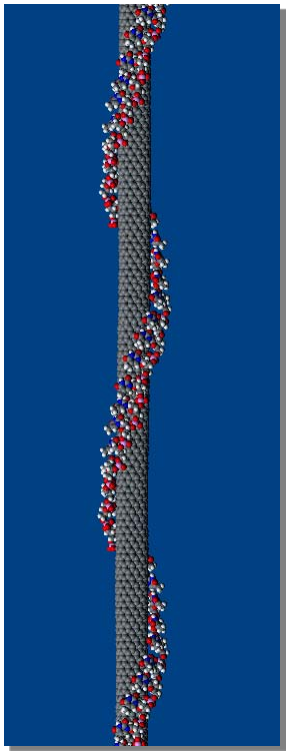
(Credit: C. Bustamante, UCBerkeley)

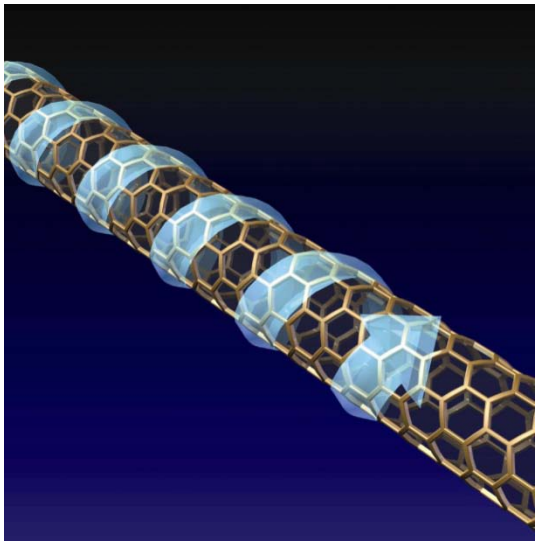
A Potential Quantum Dot Building Block For Electronics Applications

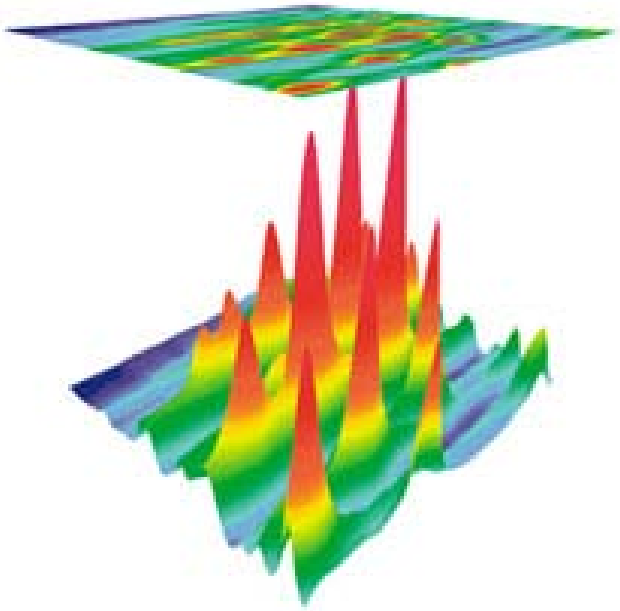


- Left: Lithographically-patterned coupled quantum dot molecule formed in a GaAs/AlGaAs heterostructure. Using voltages applied to the gates, a double-well potential is created where individual electrons can be trapped in the left or right hand well. The charge state of the molecule is read out using the quantum point contact of the confining gates as a sensor. Right: Measured “phase diagram” of the molecule, where (nL,nR) indicates the number of electrons in the left and right wells. The slanted lines indicate places where the charge state changes. (Credit: C. Marcus, Harvard U.)

Carbon Nanotubes - a Prototype 1D (one-dimensional) material of the Nanoworld

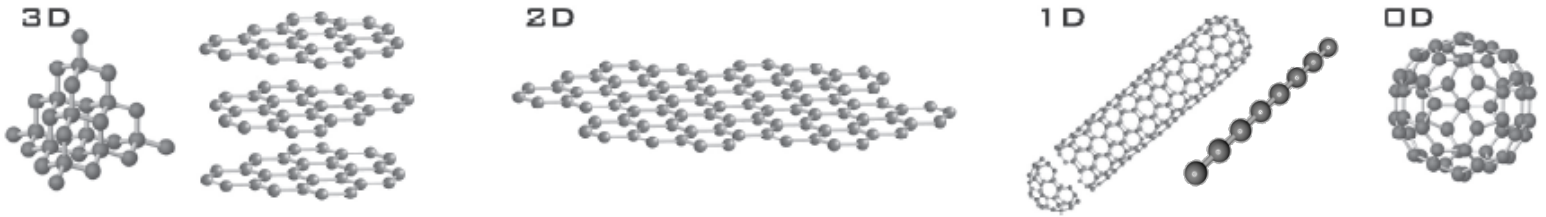




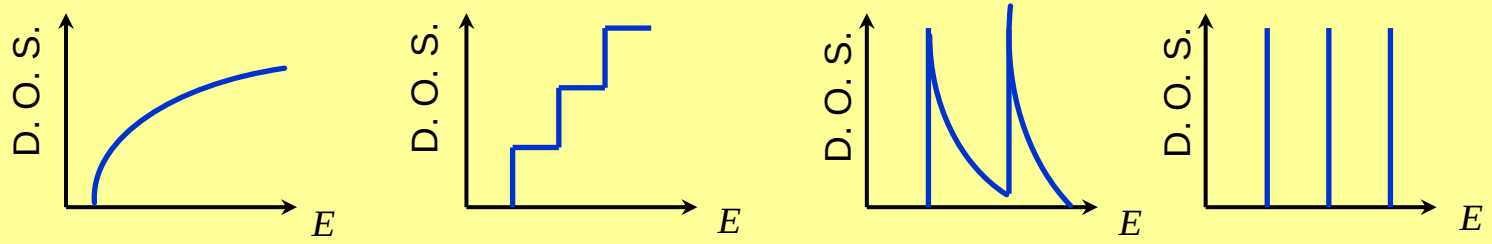


Left: Electron spiraling down a nanotube. The nanotube energy levels are quantized, as in an atom, so that every (n,m) nanotube species has a different fluorescence peak energy determined by its diameter and chirality, as shown in the right panel. (Credits: left, P. McEuen, Cornell U; right, R.B. Weisman, Rice U)

Carbon Allotropes with various dimensions



Diamond graphite graphene nanotube nanowire fullerene



3D
Bulk Semiconductor

2D
Quantum Well

1D
Quantum Wire

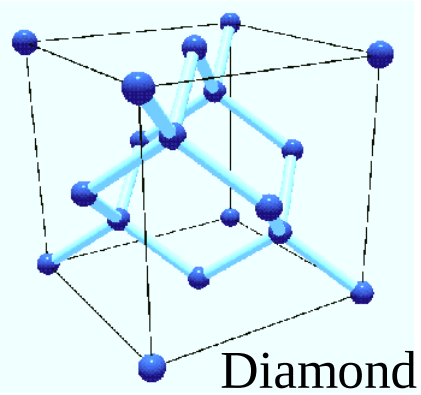
0D
Quantum Dot

Hill, J. W., and Petrucci, R. H., *General Chemistry*, 3rd edition, Prentice Hall, NJ, (2002)

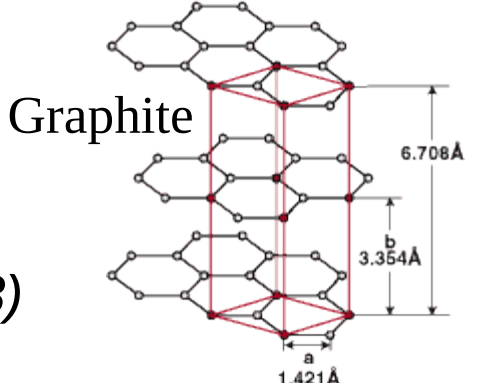
Family of carbon

hybridization and geometry

R. Saito, *in "Carbon Alloy" Elsevier (2003)*



Diamond



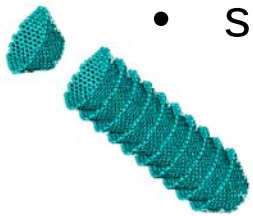
Graphite

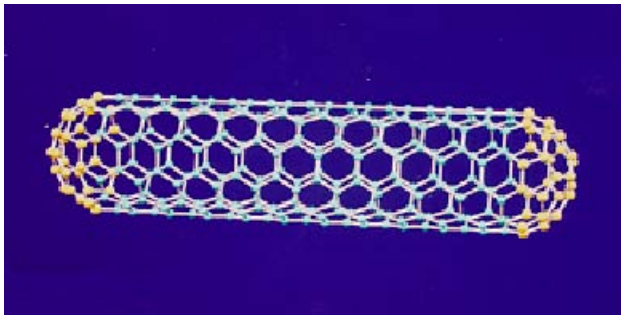
Fullerene

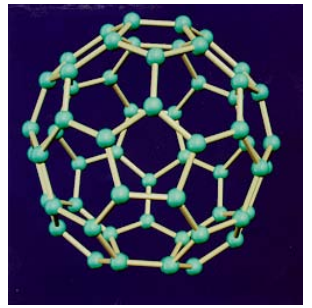
- sp^3: Diamond (3D)
- sp^2: Graphite (2D)

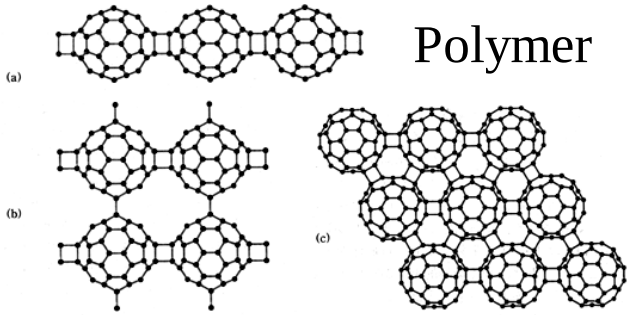
  Fullerene (0D)

  Fullerene Polymer(1-3D)
  Nanotube (1D)
  Peapod (0D+1D)
- sp: Carbyne (1D)
- Not crystal: HOPG, VGCF, glassy, whisker, fiber, nanohorn, turbostratic, ribbon

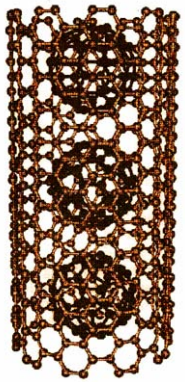


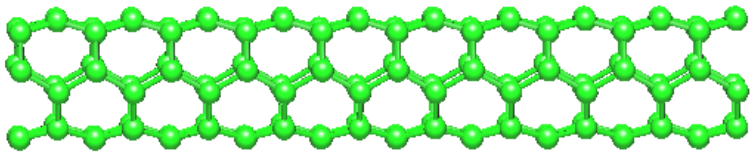




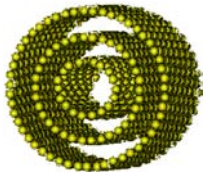


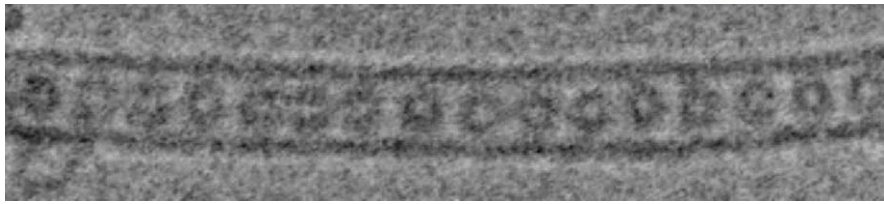
Polymer





ribbon



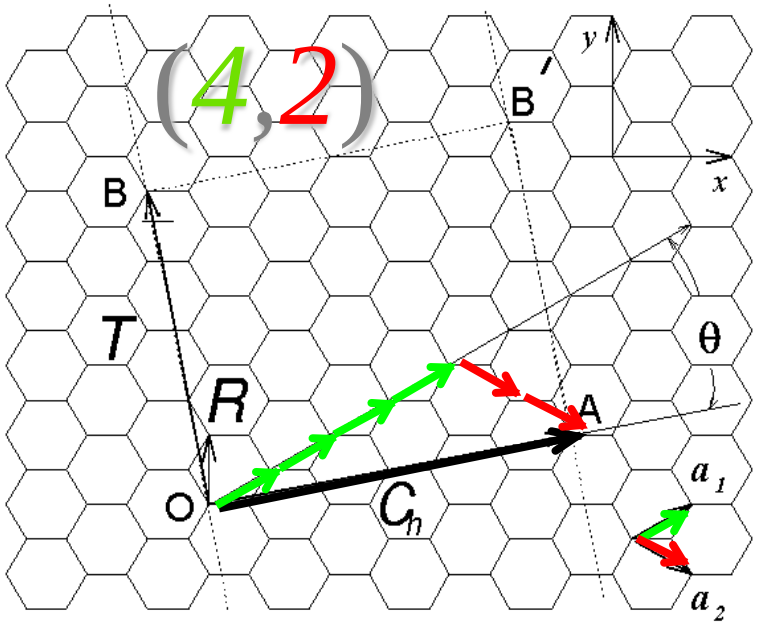


Peapod

Nanotube Structure

Rolling graphene into a cylinder

Chiral vector: $\boldsymbol{C_h} = n\boldsymbol{a_1} + m\boldsymbol{a_1} \equiv (n,m)$



Physical properties depend on (n,m):

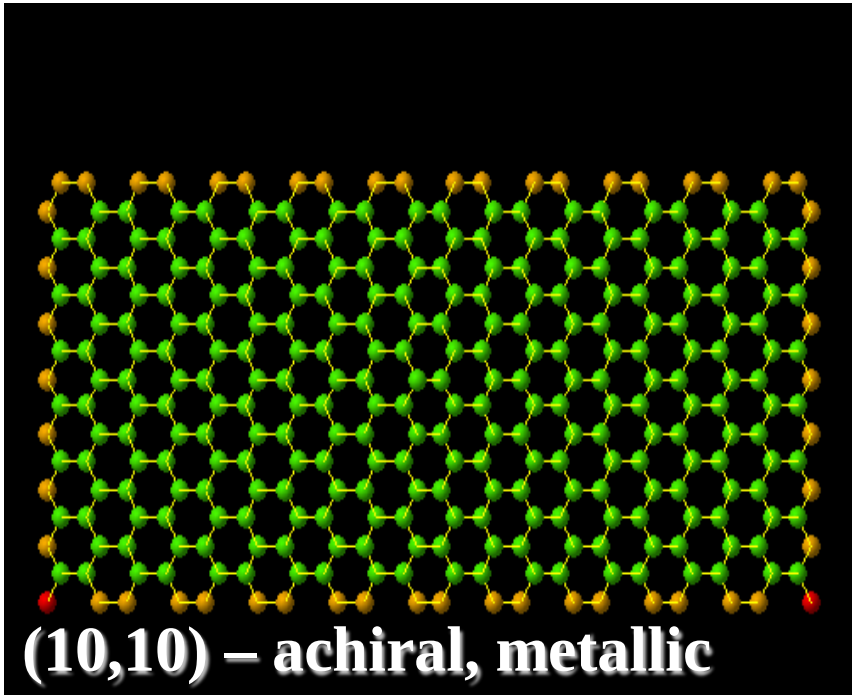
Diameter

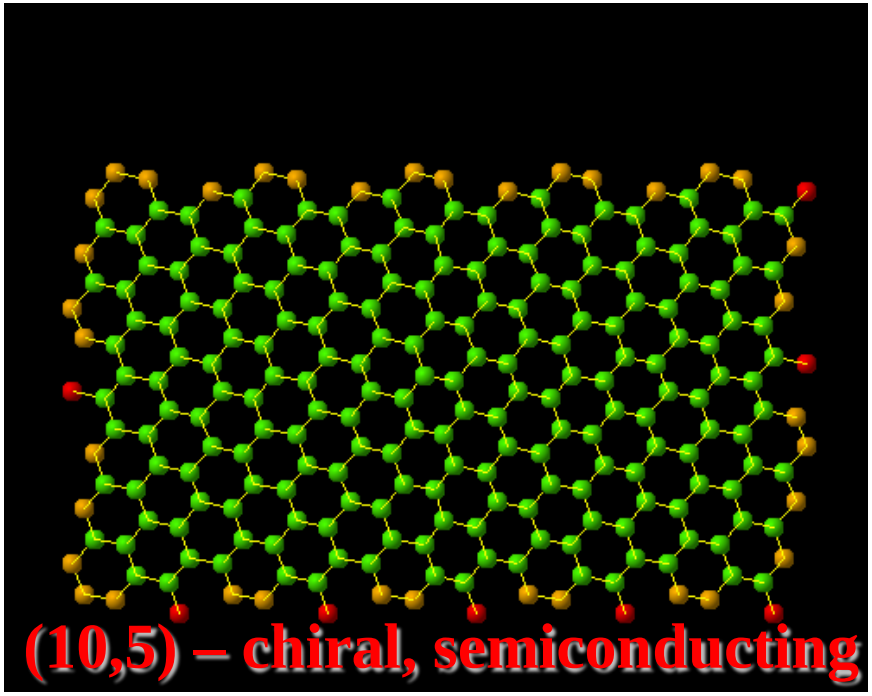
$$d_t = \sqrt{3}a_{C-C}(n^2 + m^2 + nm)^{1/2} / \pi$$

Chirality

$$\theta = \tan^{-1}\left(\frac{\sqrt{3}m}{2n+m}\right)$$

$$n - m = \begin{cases} 3p & \text{metal} \\ 3p \pm 1 & \text{semiconductor} \end{cases}$$

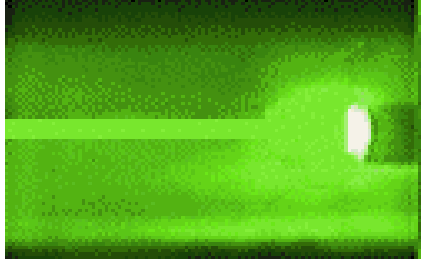




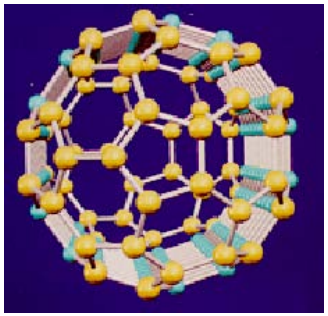
Arc Method:(by Y. Saito)

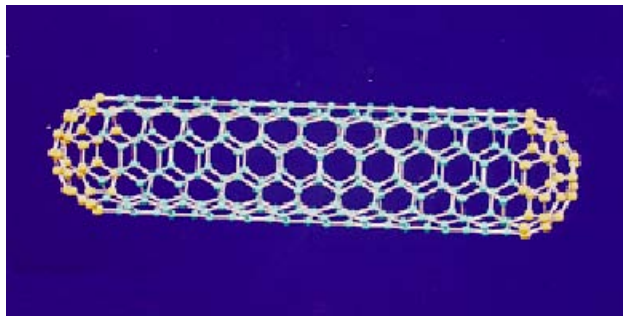
18 years of Carbon Nanotubes

S. Iijima, (1991), M. S. Dresselhaus *et al.* (1991)
J. Mintmire *et al.*, R. Saito *et al.*, N. Hamada *et al*, K. Tanaka *et al*,



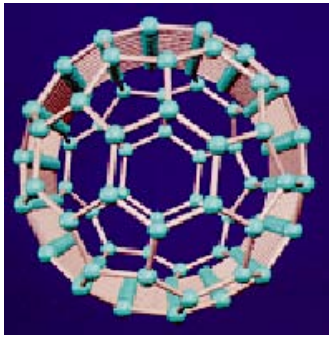
Laser Ablation:(by H. Kataura)

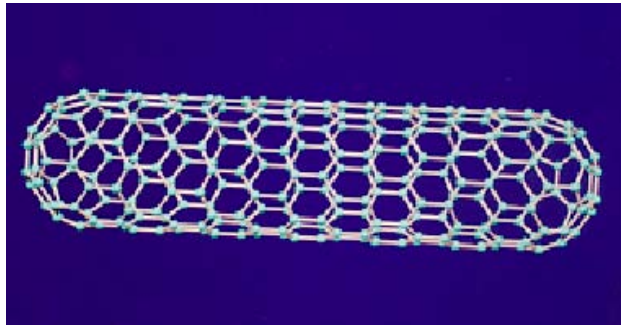




(5,5)

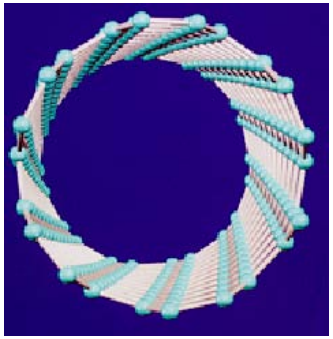
Armchair Nanotube

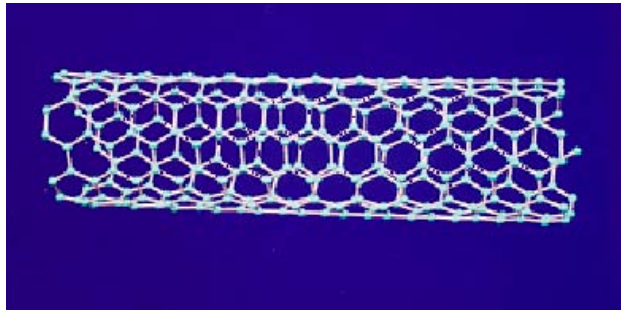




(9,0)

Zigzag Nanotube



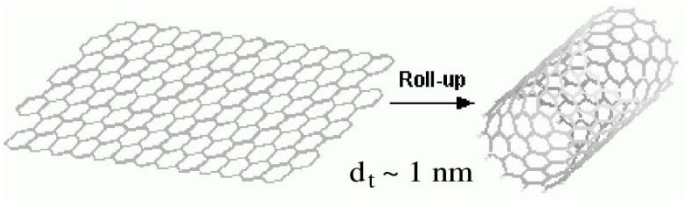


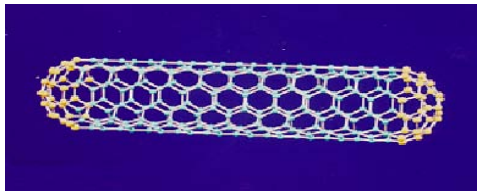
(6,5)

Chiral Nanotube

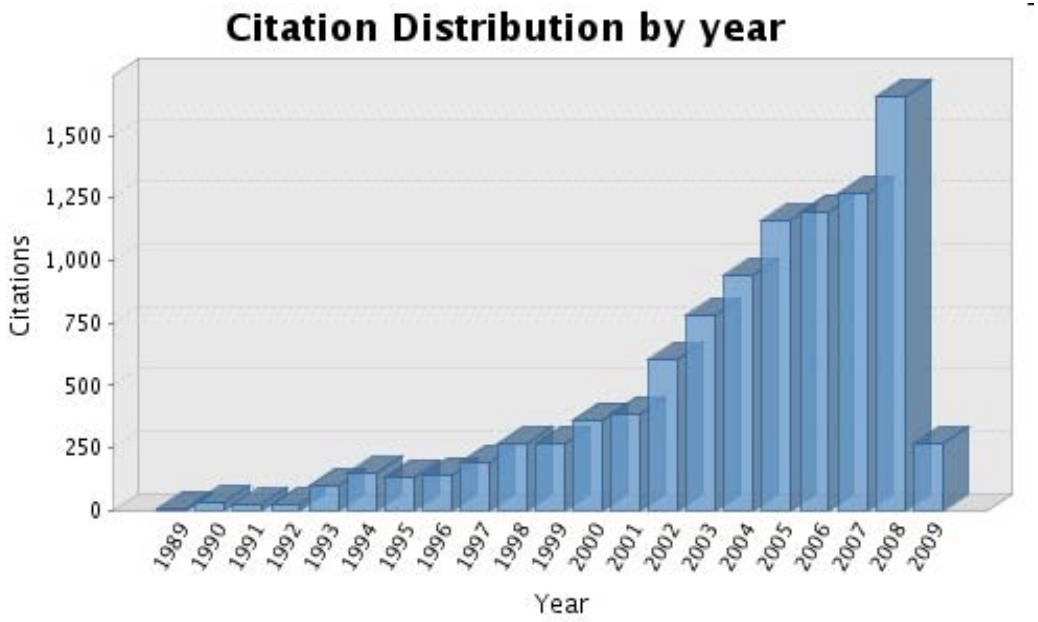
Carbon Nanotubes & Graphene
both are rapidly growing fields

- ***Nanotube publications go back to 1952***
- ***Graphene publications go back to 1947***
- ***Number of nanotube publications is still growing rapidly***





1993 SWNT

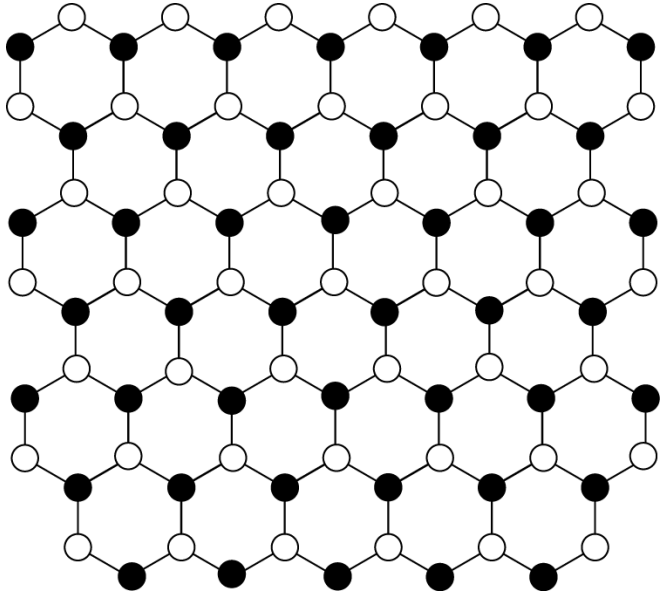


number of publications containing “Carbon Nanotube” vs. time

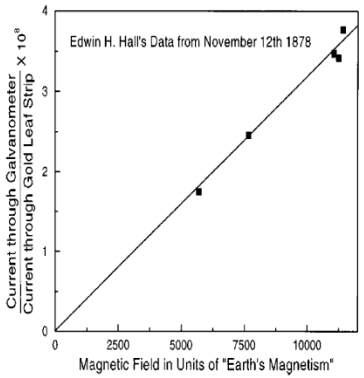
Why *now* graphene?

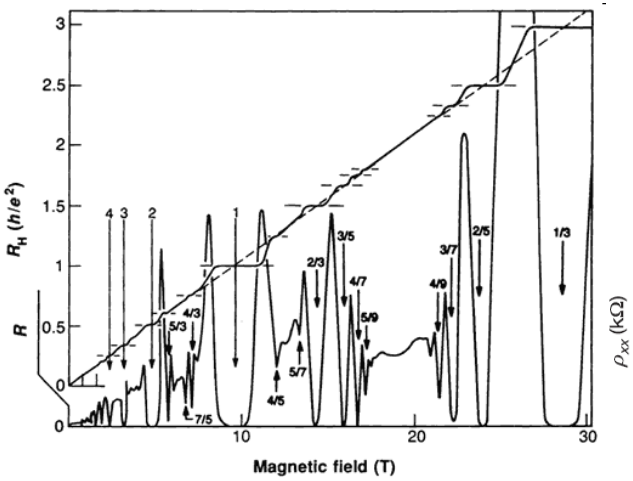
- High performance nano-device
  - high mobility 100,000cm^2/Vs at 300K
  - Improvement of nanotechnology
  - Fabricated easier than nanotubes
  - Long spin coherence μm
  - Exotic physics (QHE) at 300K
  - Stable, chemically inactive
- Challenge for graphene devices
  - Integration, process technique
  - Synthesis (SiC, CVD, Scotch tape)
  - Opening energy gap, Edges, defects

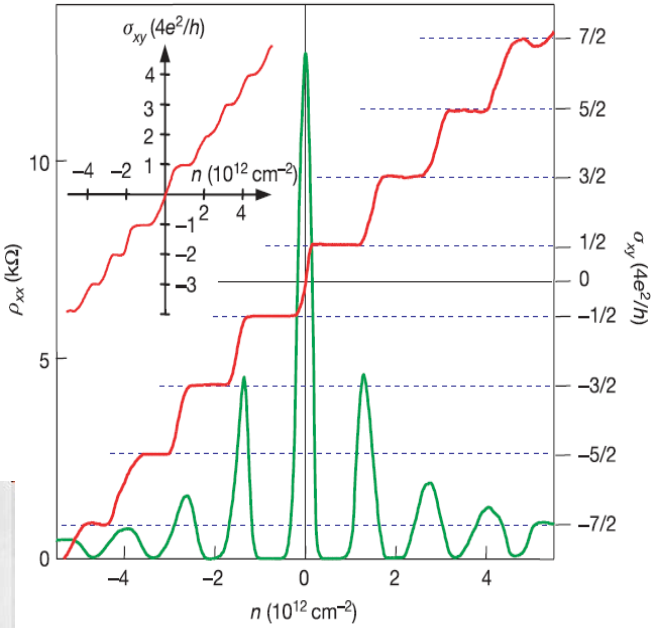
Graphene
= single layer of graphite
= 2D graphite

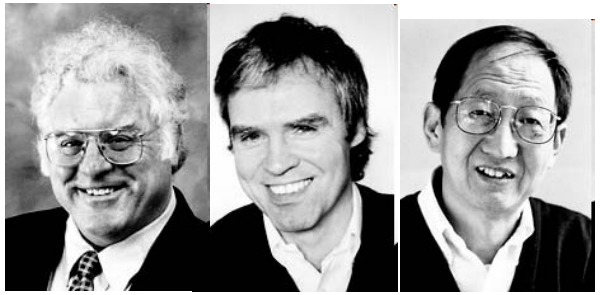


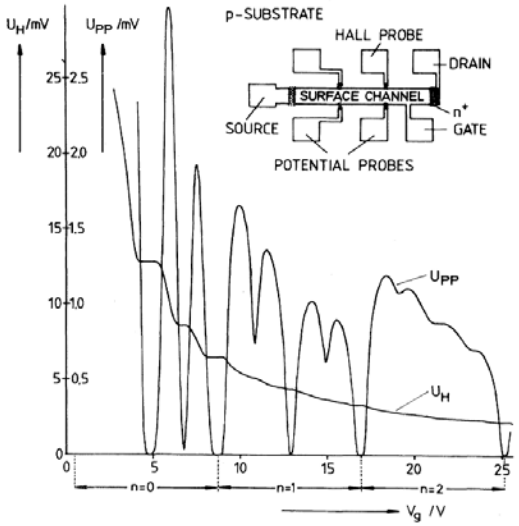
Quantum Hall Effect of Graphene





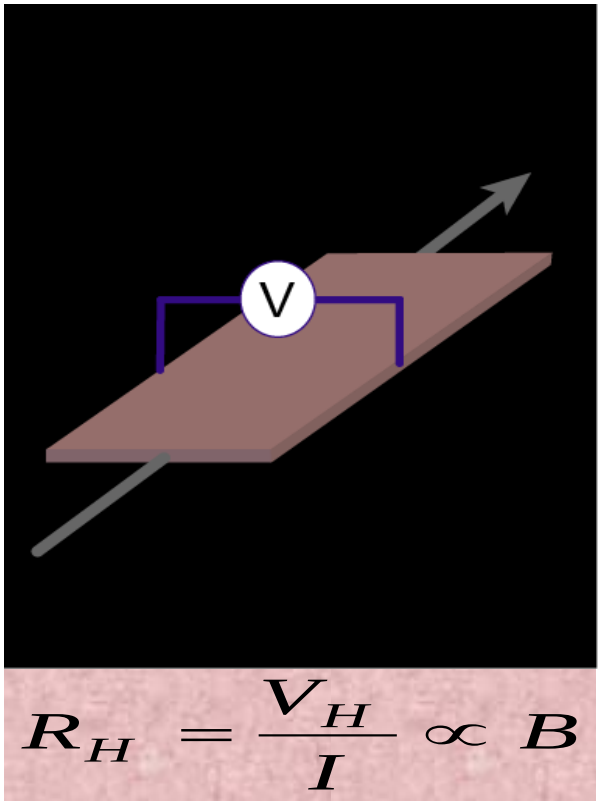




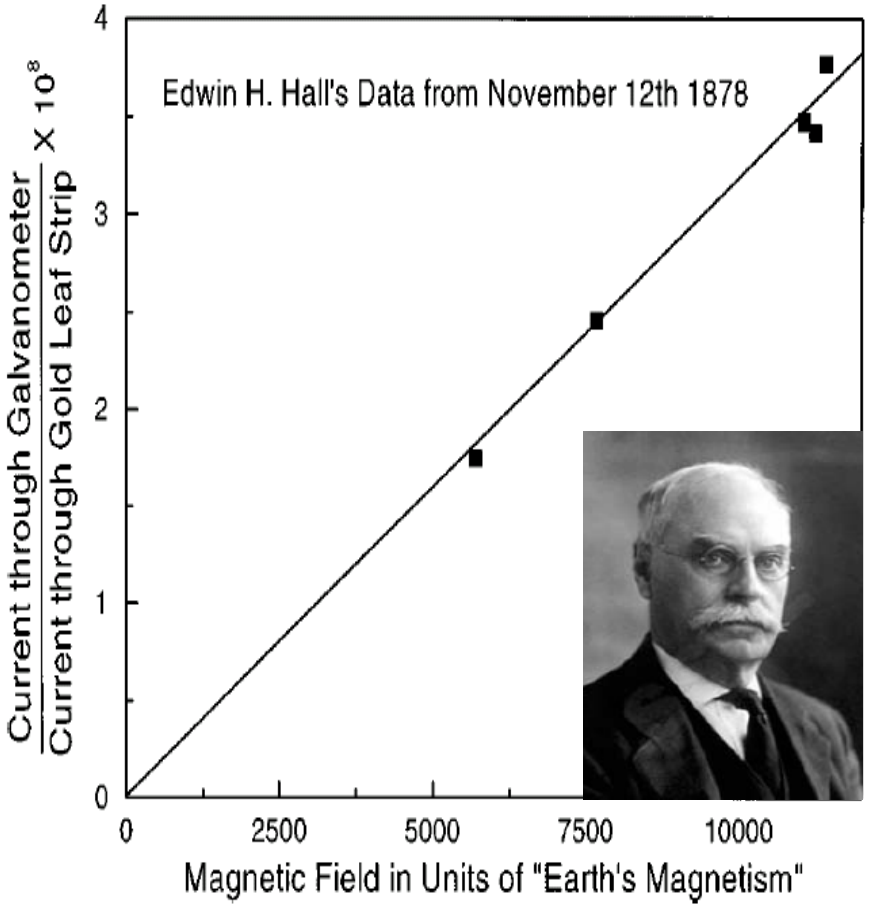


Hall Effect in 1878

In a magnetic field



$$R_H = \frac{V_H}{I} \propto B$$



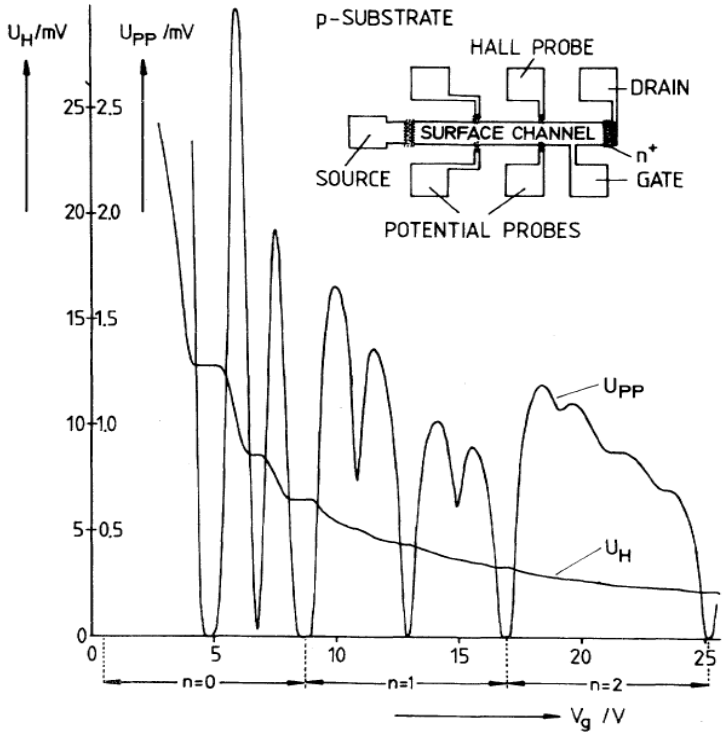
Quantum Hall Effect in 1980

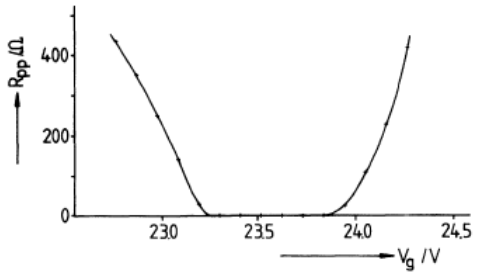
VOLUME 45, NUMBER 6 PHYSICAL REVIEW LETTERS 11 AUGUST 1980

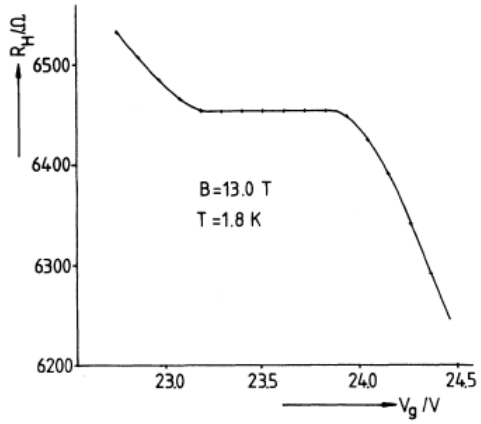
New Method for High-Accuracy Determination of the Fine-Structure Constant Based on Quantized Hall Resistance

K. v. Klitzing

Physikalisches Institut der Universität Würzburg, D-8700 Würzburg, Federal Republic of Germany, and Hochfeld-Magnetlabor des Max-Planck-Instituts für Festkörperforschung, F-38042 Grenoble, France



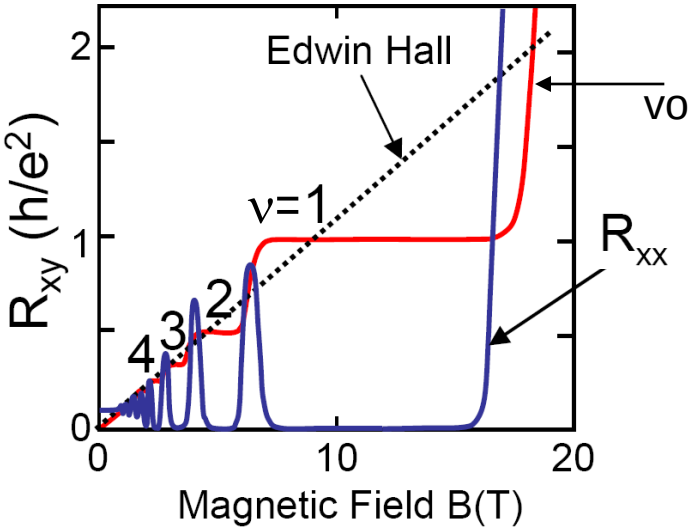




$$\rho_{xy} = \frac{h}{ie^2},$$

Quantum Hall Effect

(Classical) Hall effect



Quantum Hall effect

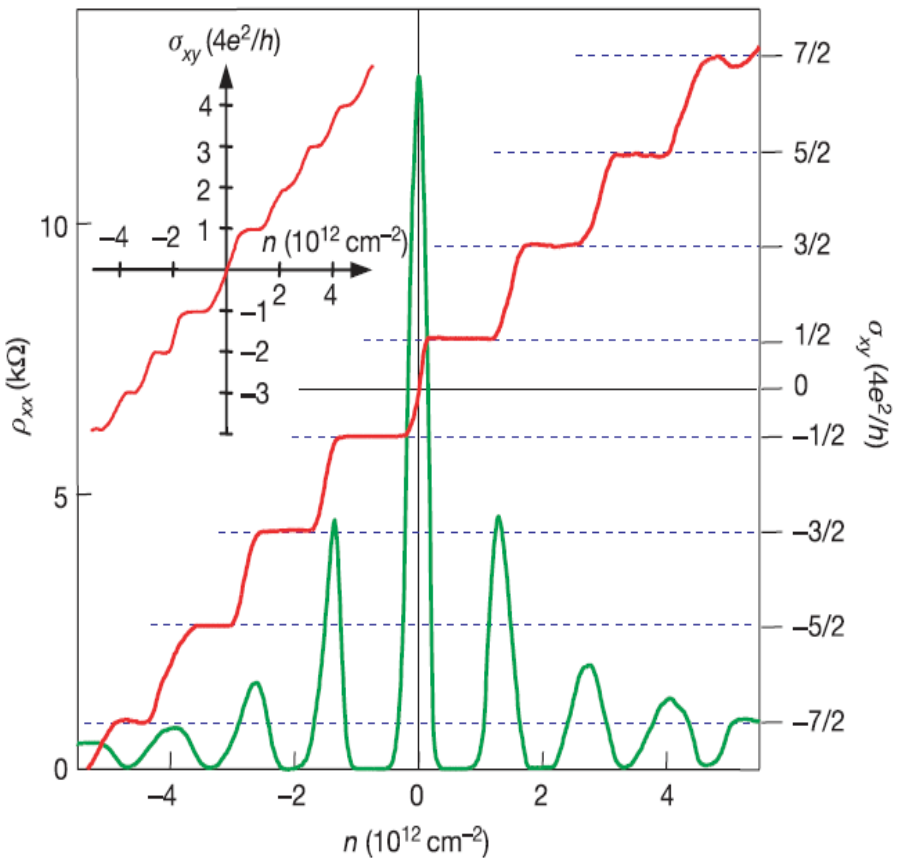
$$\sigma_{xy} = R_{xy}^{-1} = n \frac{e^2}{h}$$

Landau level Filling factor ν

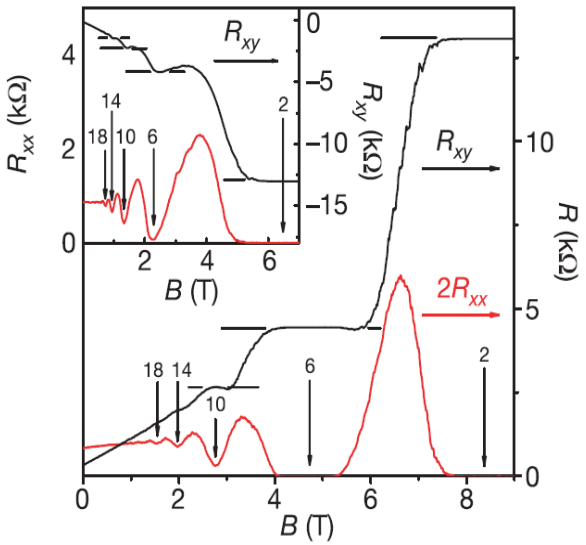
$$\nu \equiv \frac{N}{N_\phi} = \frac{2\pi\hbar}{eB} n = 2\pi \ell_B^2 n$$

QHE of Graphene in 2005

$$\sigma_{yx} = (n + 1/2)\ [4e^2/h]$$



Nature 438 (2005) 04233, 04235



Half-integer quantum Hall effect

Zheng-Ando, Gusynin-Sharapov, Peres et al.

Additional Quantum Hall Plateaus

PRL **96,** 136806 (2006) PHYSICAL REVIEW LETTERS week ending 7 APRIL 2006

Landau-Level Splitting in Graphene in High Magnetic Fields

Y. Zhang,[1] Z. Jiang,[1,3] J. P. Small,[1] M. S. Purewal,[1] Y.-W. Tan,[1] M. Fazlollahi,[1] J. D. Chudow,[1]
J. A. Jaszczak,[4] H. L. Stormer,[1,2] and P. Kim[1]

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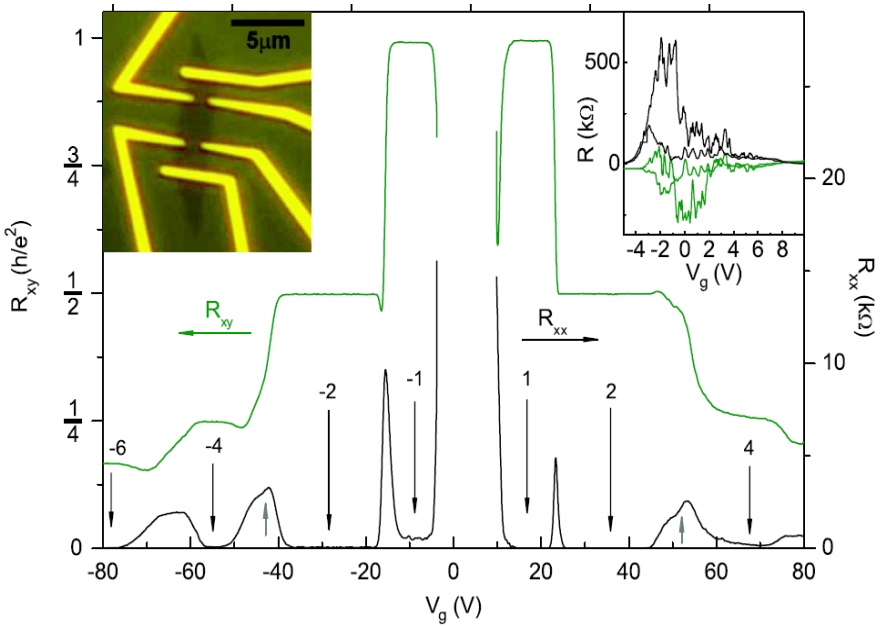
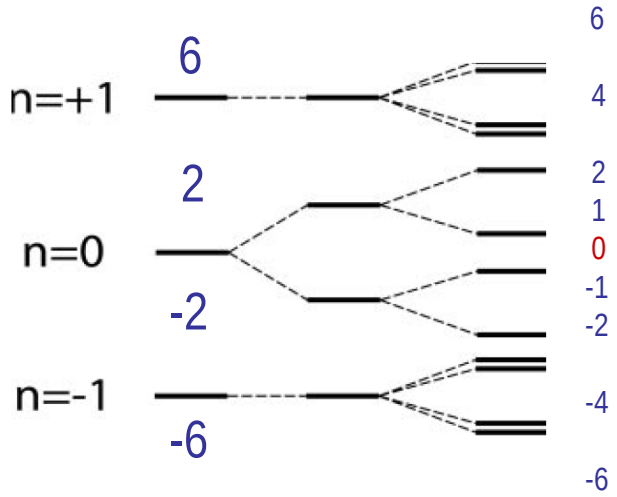
[2]*Bell Labs, Lucent Technologies, Murray Hill, New Jersey 07974, USA*
[3]*National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA*
[4]*Department of Physics, Michigan Technological University, Houghton, Michigan 49931, USA*

(Received 1 January 2006; published 6 April 2006)





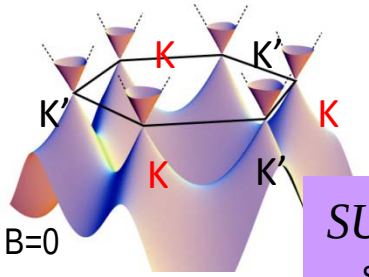
Valley and spin splitting in the strong field limit

Graphene Quantum Hall Ferromagnet

PRL 96, 256602 (2006) PHYSICAL REVIEW LETTERS week ending 30 JUNE 2006

Quantum Hall Ferromagnetism in Graphene

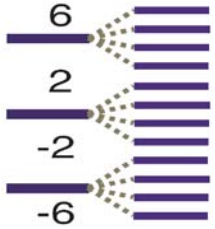
Kentaro Nomura and Allan H. MacDonald
Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081, USA
(Received 4 April 2006; published 28 June 2006)



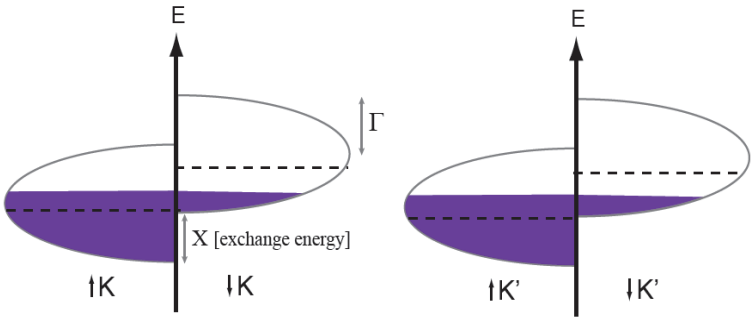
$$SU(2) \otimes SU(2) = SU(4)$$
spin valley

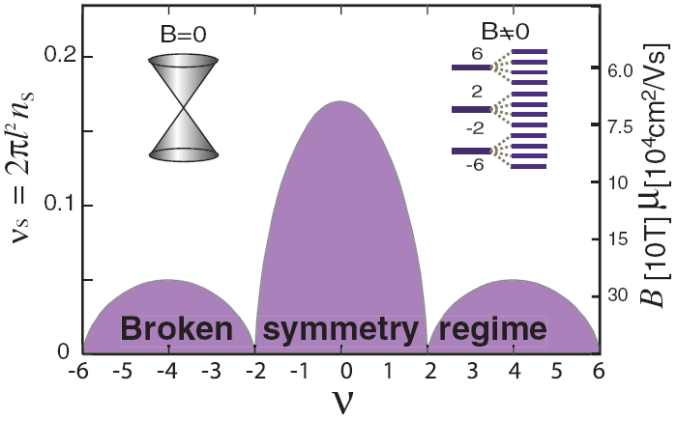
disordered [weak B] clean [strong B]

$E_C << \Gamma$



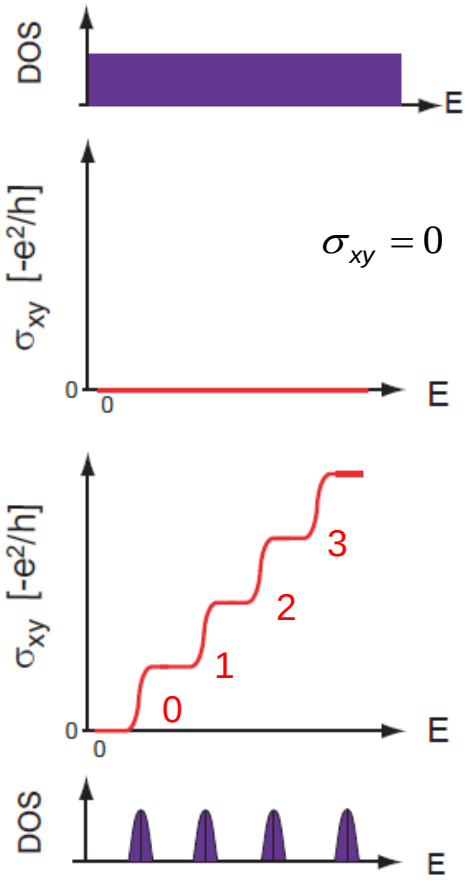
$E_C >> \Gamma$





QHE in zero-field limit

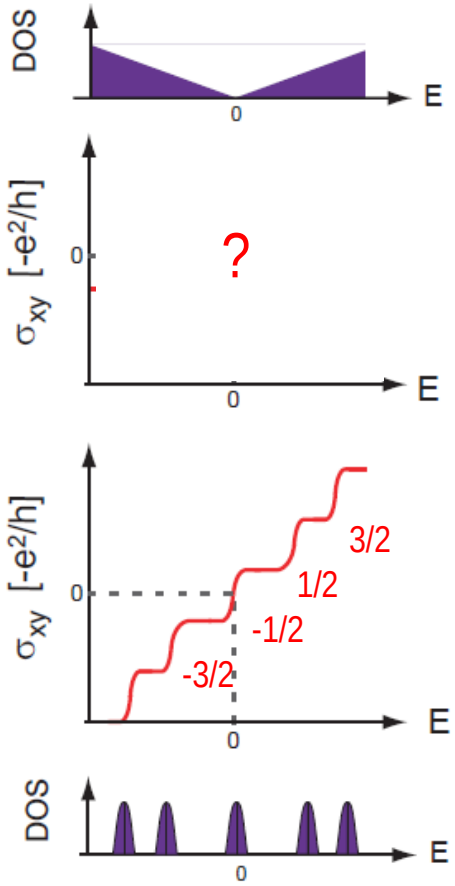
"Non-relativistic"



weak B field
(strong disorder)

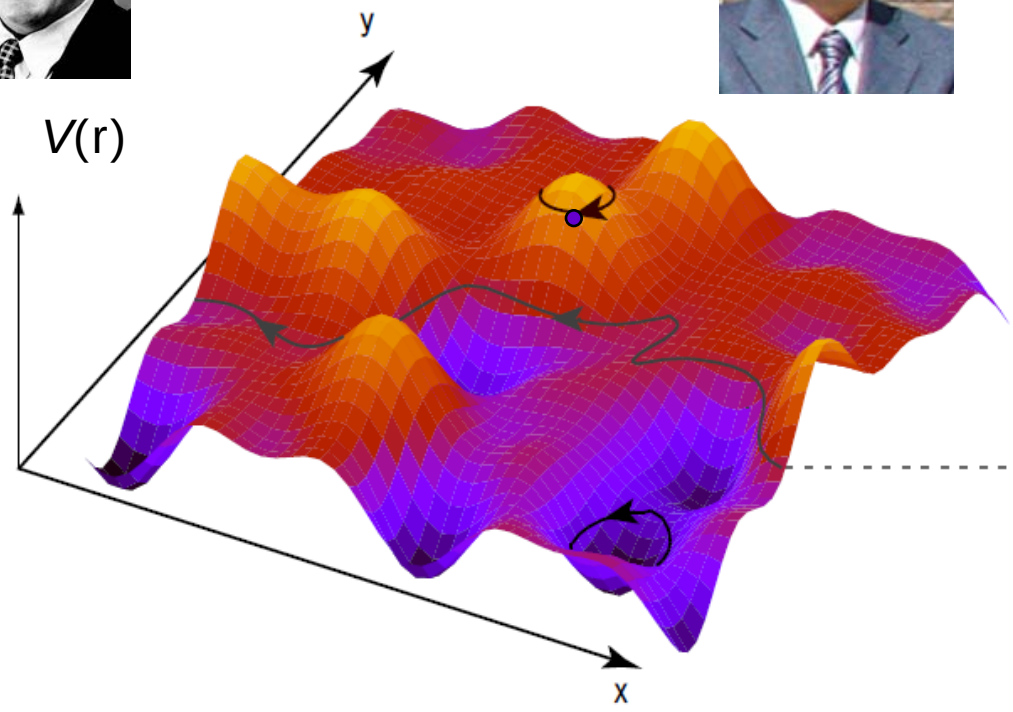
strong B field
(weak disorder)

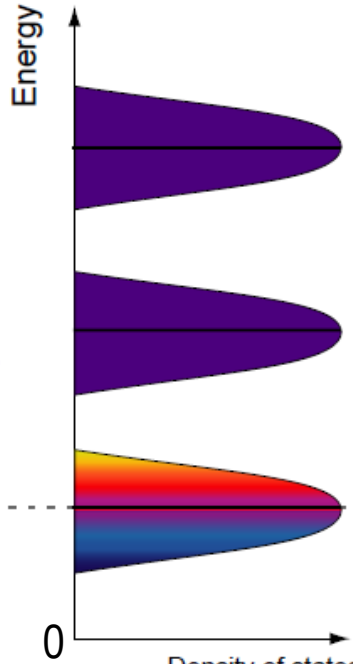
"Relativistic"

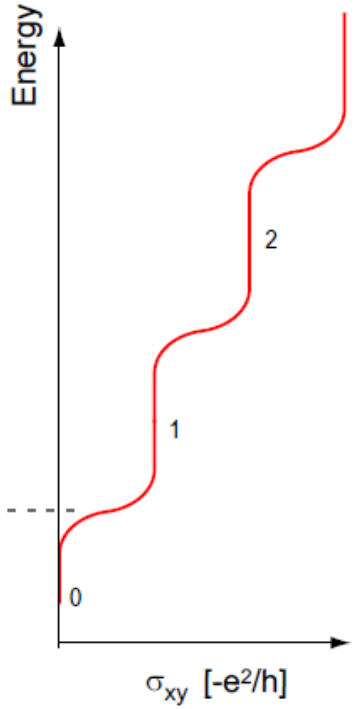


QHE: Localization in B-fields

$$H = \frac{(\mathbf{p} - e\mathbf{A}(\mathbf{r}))^2}{2m} + V(\mathbf{r})$$

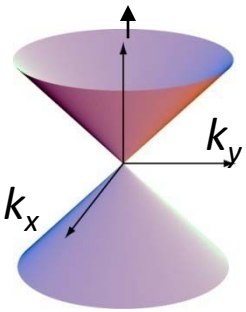






Localization and QHE

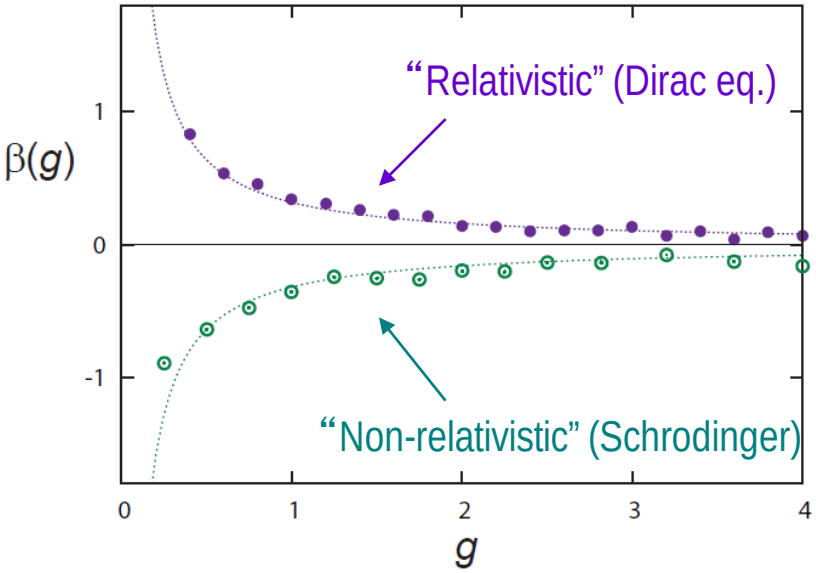
Topological metal



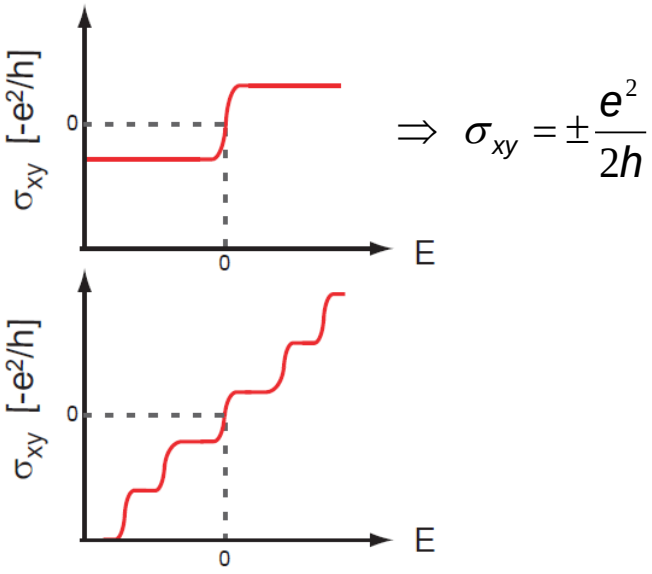
massless Dirac fermions

QHE in a vanishing B-field

$B = 0$



$B \neq 0$



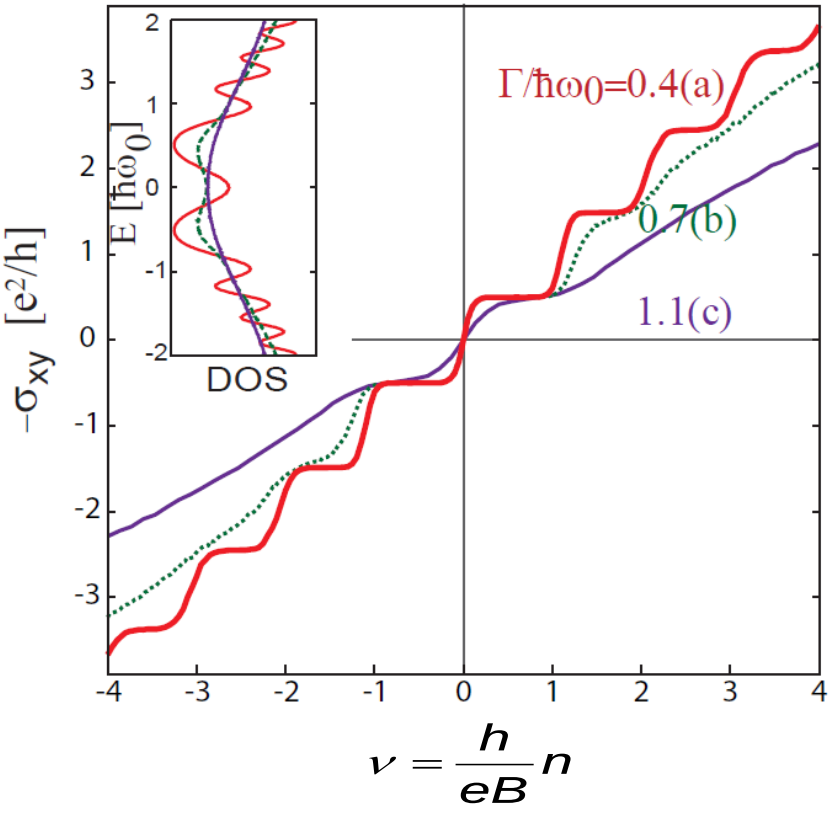
$$\Rightarrow \sigma_{xy} = \pm \frac{e^2}{2h}$$

Singularity at Dirac point

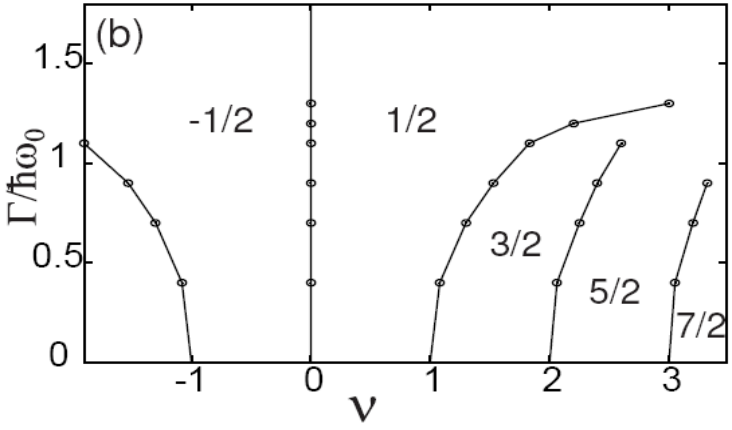
K-K' decoupled case (long-range potential)

QHE of Dirac fermions in $B \to 0$ $\quad \Rightarrow \quad \sigma_{xy} = \pm \dfrac{e^2}{2h}$

(per valley, per spin)



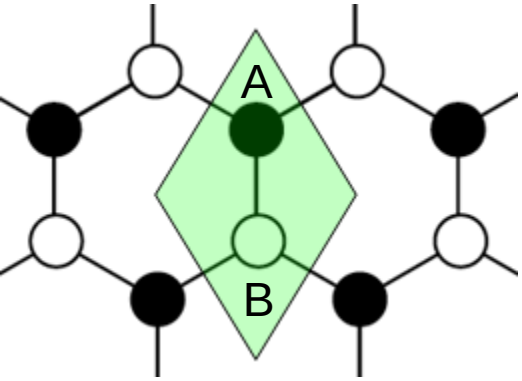
Phase diagram



Phys. Rev. Lett. 100, 246806 (2008)

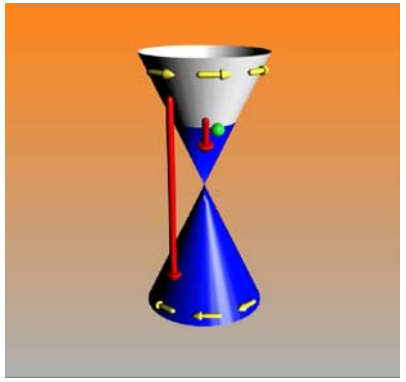
Why are nanotube and graphene special?

1. Quantum effect at 300K
2. Constant Fermi velocity $v_F = c/300$
3. Large variety of geometries more than 300.

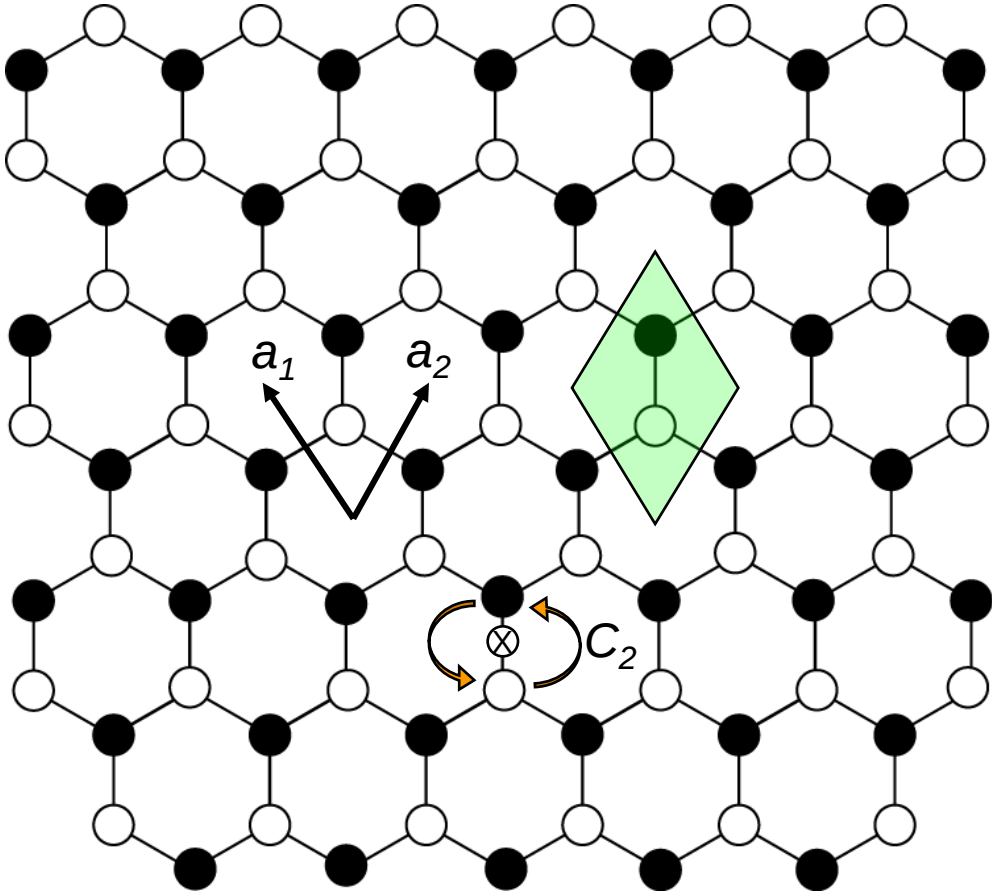


Hexagons make graphene special.

Similarity to elementary particle physics



A and B carbon atoms in graphene

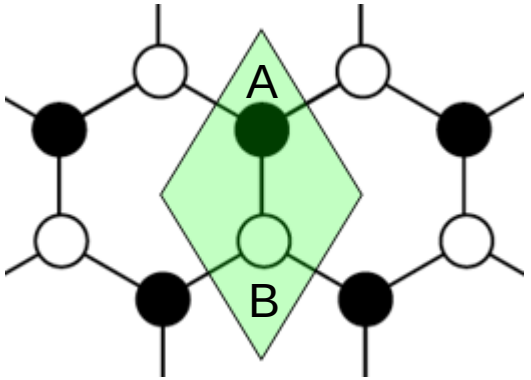


Lattice Structure of Graphene
2 fold symmetry between A and B

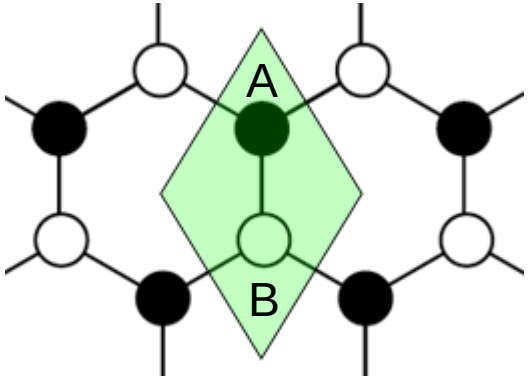
Two component wave function

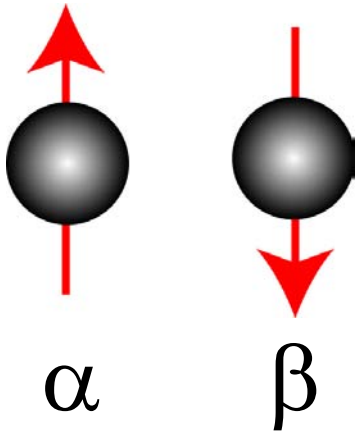
$$\Psi(\mathbf{r}) = \begin{pmatrix} \Psi_{\mathrm{A}}(\mathbf{r}) \\ \Psi_{\mathrm{B}}(\mathbf{r}) \end{pmatrix}$$

Pseudo spin



Pseudo Spin vs Real Spin





$$\Psi(\mathbf{r}) = \begin{pmatrix} \Psi_{\mathrm{A}}(\mathbf{r}) \\ \Psi_{\mathrm{B}}(\mathbf{r}) \end{pmatrix}$$

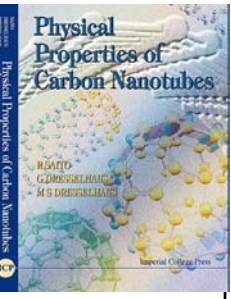
$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ only A site

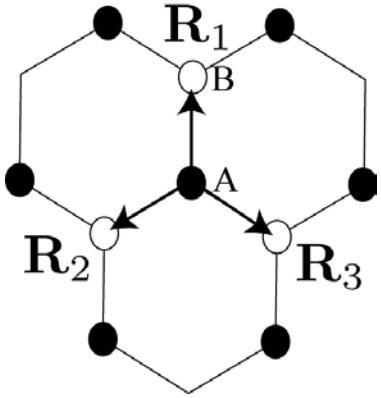
$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ only B site

$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ up spin

$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ down spin

Energy Band of Graphene





Tight Binding Hamiltonian

$$\mathcal{H} = \begin{pmatrix} \langle \Psi_A|\mathcal{H}|\Psi_A\rangle & \langle \Psi_A|\mathcal{H}|\Psi_B\rangle \\ \langle \Psi_B|\mathcal{H}|\Psi_A\rangle & \langle \Psi_B|\mathcal{H}|\Psi_B\rangle \end{pmatrix} = \begin{pmatrix} 0 & -\gamma_0 \left(e^{i\mathbf{k}\cdot\mathbf{R}_1} + e^{i\mathbf{k}\cdot\mathbf{R}_2} + e^{i\mathbf{k}\cdot\mathbf{R}_3}\right) \\ -\gamma_0 \left(e^{-i\mathbf{k}\cdot\mathbf{R}_1} + e^{-i\mathbf{k}\cdot\mathbf{R}_2} + e^{-i\mathbf{k}\cdot\mathbf{R}_3}\right) & 0 \end{pmatrix}$$

$f(\mathbf{k})$

Schrodinger Eq.

$$E(\mathbf{k}) \begin{pmatrix} \Psi_A(\mathbf{k}) \\ \Psi_B(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} 0 & -\gamma_0 f(\mathbf{k}) \\ -\gamma_0 f(\mathbf{k})^* & 0 \end{pmatrix} \begin{pmatrix} \Psi_A(\mathbf{k}) \\ \Psi_B(\mathbf{k}) \end{pmatrix}$$

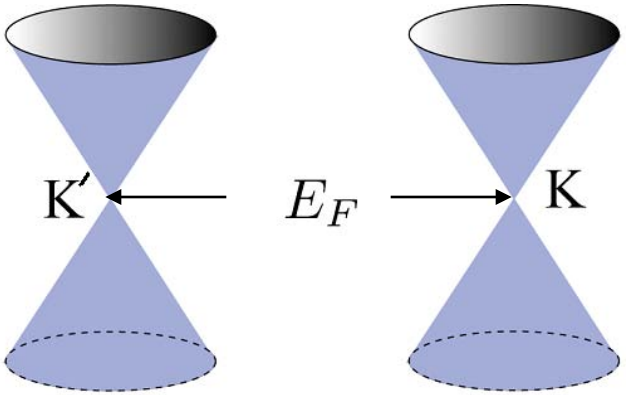
$$\det \begin{pmatrix} E(\mathbf{k}) & \gamma_0 f(\mathbf{k}) \\ \gamma_0 f(\mathbf{k})^* & E(\mathbf{k}) \end{pmatrix} = 0$$

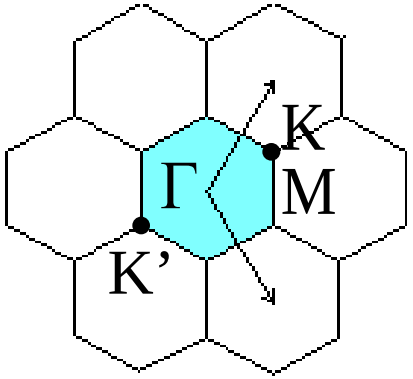
Conduction band

$$E(\mathbf{k}) = \pm\gamma_0 |f(\mathbf{k})|$$

Valence band

K and K' : Dirac points





$f(\mathbf{k}_F) = 0$ K point

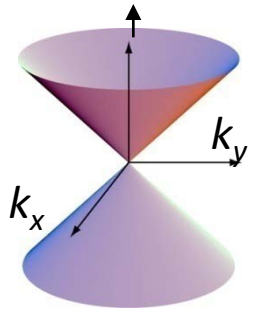
$f(-\mathbf{k}_F) = 0$ K' point

Taylor expansion of f(k) around the K point

$$E(\mathbf{k})\begin{pmatrix}\Psi_A(\mathbf{k})\\ \Psi_B(\mathbf{k})\end{pmatrix}=\begin{pmatrix}0 & -\gamma_0 f(\mathbf{k})\\ -\gamma_0 f(\mathbf{k})^* & 0\end{pmatrix}\begin{pmatrix}\Psi_A(\mathbf{k})\\ \Psi_B(\mathbf{k})\end{pmatrix}$$

K point $f(\mathbf{k}_\mathrm{F})=0$

$$=\frac{3\gamma_0 a_{cc}}{3}\begin{pmatrix}0 & k_x-ik_y+\cdots\\ k_x+ik_y+\cdots & 0\end{pmatrix}\begin{pmatrix}\Psi_A(\mathbf{k})\\ \Psi_B(\mathbf{k})\end{pmatrix}$$



Hamiltonian around the K point

$$\mathcal{H}_\mathrm{K}=\hbar v_\mathrm{F}\begin{pmatrix}0 & k_x-ik_y\\ k_x+ik_y & 0\end{pmatrix}$$

$$v_\mathrm{F}=\frac{\gamma_0 a_{CC}}{\hbar}$$

$$k_x=|\mathbf{k}|\cos\Theta(\mathbf{k})$$
$$k_y=|\mathbf{k}|\sin\Theta(\mathbf{k})$$

$$\begin{pmatrix}0 & e^{-i\Theta}\\ e^{i\Theta} & 0\end{pmatrix}\begin{pmatrix}1\\ e^{i\Theta}\end{pmatrix}=\begin{pmatrix}1\\ e^{i\Theta}\end{pmatrix}$$

$$\begin{pmatrix}0 & e^{-i\Theta}\\ e^{i\Theta} & 0\end{pmatrix}\begin{pmatrix}1\\ -e^{i\Theta}\end{pmatrix}=-\begin{pmatrix}1\\ -e^{i\Theta}\end{pmatrix}$$

$$\mathcal{H}_\mathrm{K}=\hbar v_\mathrm{F}|\mathbf{k}|\begin{pmatrix}0 & e^{-i\Theta(\mathbf{k})}\\ e^{+i\Theta(\mathbf{k})} & 0\end{pmatrix}$$

Eigenvalue

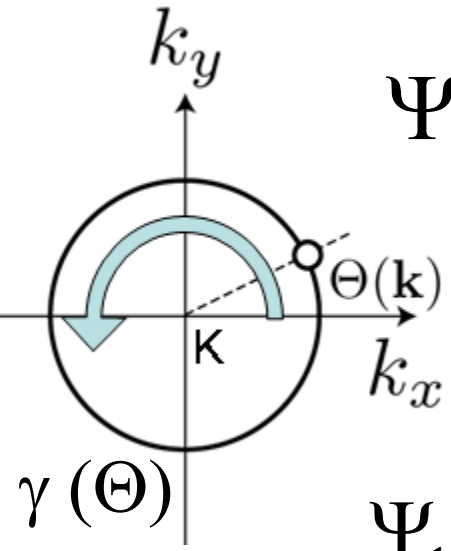
$$E(\mathbf{k})=\pm\hbar v_\mathrm{F}|\mathbf{k}|$$

Eigenvector

$$\Psi(\mathbf{k})=\begin{pmatrix}1\\ \pm e^{i\Theta}\end{pmatrix}$$

The phase of the wavefunction and Berry's phase

T. Ando et al., *J. Phys. Soc. Jpn.* **67**, 2857 (1998)



$$\Psi_1(\mathbf{k}) = \begin{pmatrix} 1 \\ e^{+i\Theta(\mathbf{k})} \end{pmatrix} \qquad \Psi_2(\mathbf{k}) = \begin{pmatrix} e^{-i\Theta(\mathbf{k})/2} \\ e^{+i\Theta(\mathbf{k})/2} \end{pmatrix}$$

$$\left(= e^{-i\Theta(\mathbf{k})/2}\Psi_1(\mathbf{k}) \right)$$

Θ: 0 2π around the K point,

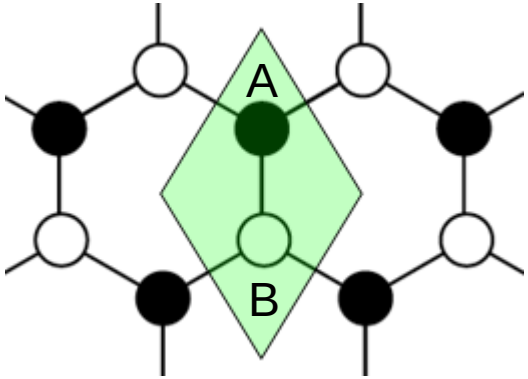
$$\Psi_1(\mathbf{k}+2\pi) = \Psi_1(\mathbf{k}) \qquad \Psi_2(\mathbf{k}+2\pi) = -\Psi_2(\mathbf{k})$$

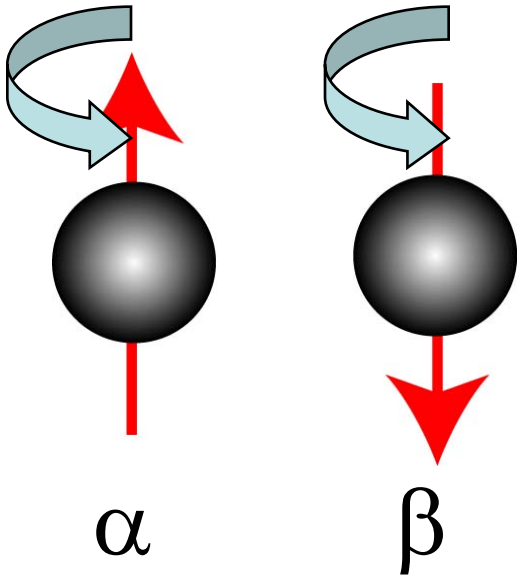
We must add the Berry Phase γ: Θ □ $\Theta+\gamma$

$$\gamma\,(\Theta) = \qquad \pi \qquad\qquad 0$$

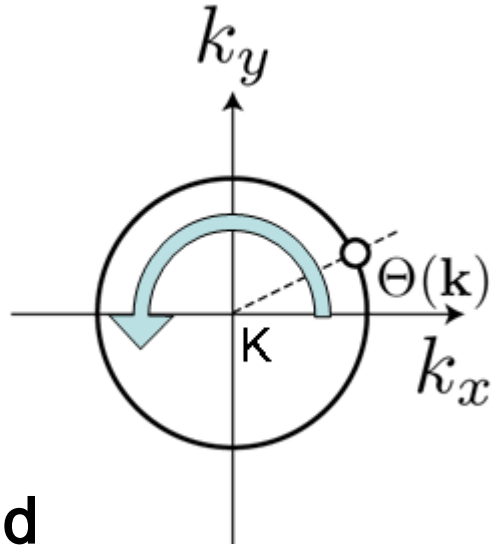
$$\Psi_1(\mathbf{k}+2\pi) = -\Psi_1(\mathbf{k}) \qquad \Psi_2(\mathbf{k}+2\pi) = -\Psi_2(\mathbf{k})$$

4 π rotational symmetry of Pseudo Spin vs Real Spin





$$\Psi(\mathbf{r}) = \begin{pmatrix} \Psi_{\mathrm{A}}(\mathbf{r}) \\ \Psi_{\mathrm{B}}(\mathbf{r}) \end{pmatrix}$$



4 π rotation in the k space

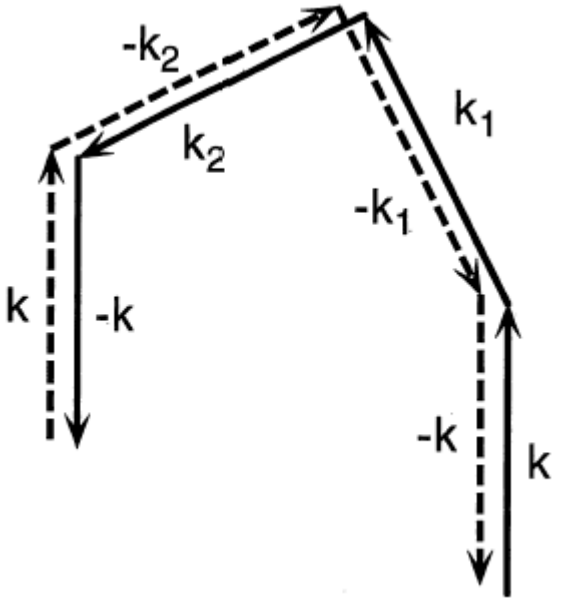
rotation around the K (K') point

4 π rotation in the real space

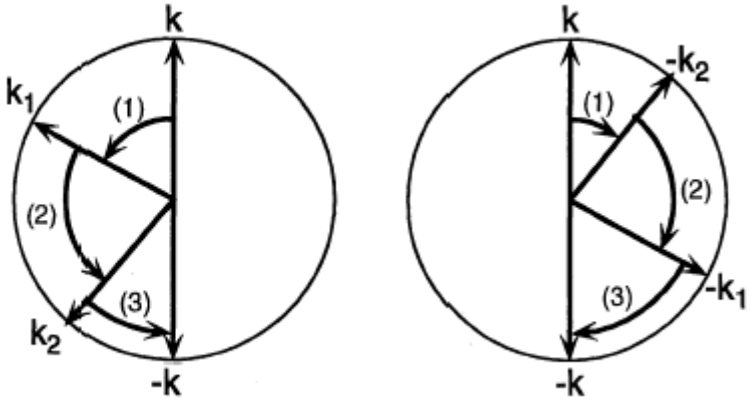
rotation around *z*-axes

Absence of Back scattering

T. Ando et al., *J. Phys. Soc. Jpn*, 67, 2857 (1998)



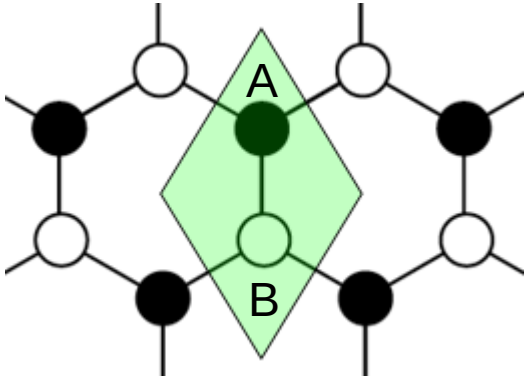
A time reversal pair of back scatterimg

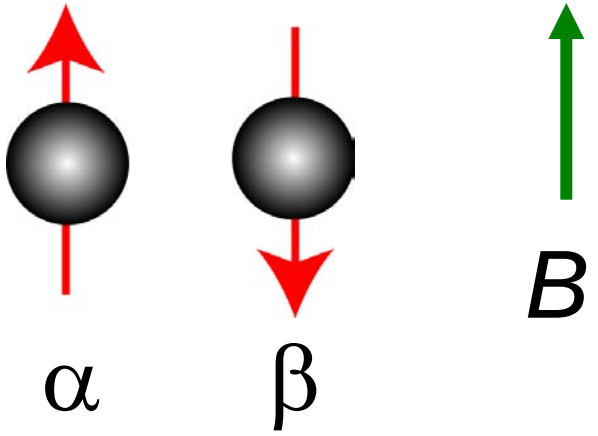


Cancel scattering amplitude

to each other by the phase difference of π.

Question: what is the field that polarizes Pseudo Spin or Real Spin?





$$\Psi(\mathbf{r}) = \begin{pmatrix} \Psi_{\mathrm{A}}(\mathbf{r}) \\ \Psi_{\mathrm{B}}(\mathbf{r}) \end{pmatrix}$$

$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ only A site

$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ only B site

A: Magnetic field *B*

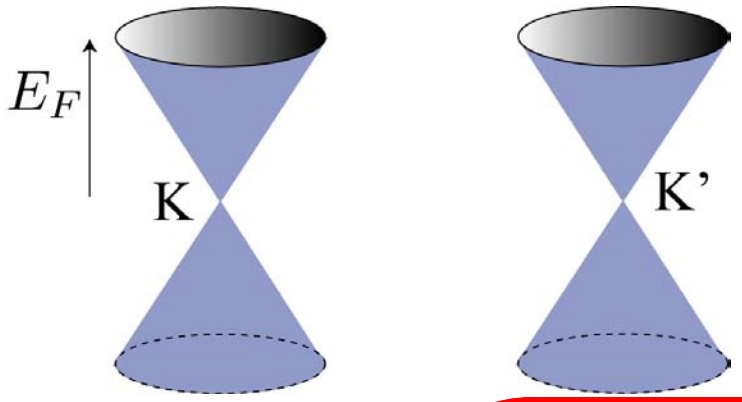
$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ up spin

$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ down spin

Effective Hamiltonian around the K point

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$



$$E(\mathbf{k}) = \pm\hbar v_{\mathrm{F}}|\mathbf{k}|$$

K point

$$\mathcal{H}_{\mathrm{K}} = \hbar v_{\mathrm{F}} \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix}$$

$$\boldsymbol{\sigma} \cdot \mathbf{p} = \sigma_x p_x + \sigma_y p_y$$

$$\mathcal{H}_{\mathrm{K}} = v_{\mathrm{F}} \boldsymbol{\sigma} \cdot \hat{\mathbf{p}}$$

K'point

$$\mathcal{H}_{\mathrm{K}'} = \hbar v_{\mathrm{F}} \begin{pmatrix} 0 & -k_x - ik_y \\ -k_x + ik_y & 0 \end{pmatrix}$$

$$\boldsymbol{\sigma}' = (-\sigma_x, \sigma_y)$$

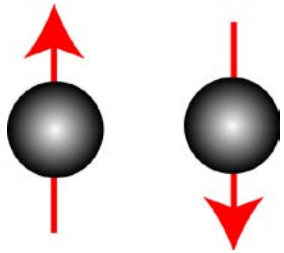
$$\boldsymbol{\sigma}' \cdot \mathbf{p} = -\sigma_x p_x + \sigma_y p_y$$

$$\mathcal{H}_{K'} = v_{\mathrm{F}} \boldsymbol{\sigma}' \cdot \hat{\mathbf{p}}$$

Dirac's equation

$$E\begin{pmatrix}\Psi_L\\ \Psi_R\end{pmatrix}=\begin{pmatrix}-c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}} & mc^2I\\ mc^2I & c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\end{pmatrix}\begin{pmatrix}\Psi_L\\ \Psi_R\end{pmatrix}$$

Mass



$$\begin{pmatrix}\Psi_L^{\uparrow}\\ \Psi_L^{\downarrow}\\ \Psi_R^{\uparrow}\\ \Psi_R^{\downarrow}\end{pmatrix}$$

Paul Adrien Maurice Dirac
1902.8.8-1984.10.20

Hamiltonian of a relativistic electron with electronic real spin

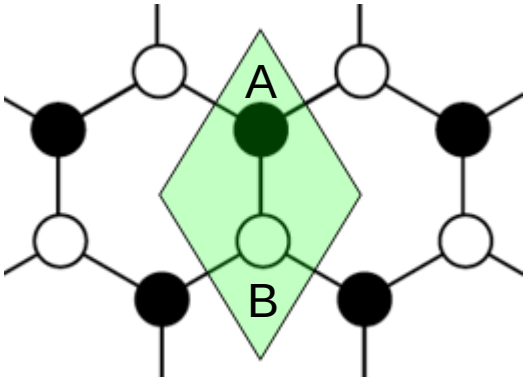
When *m=0*

$$\mathcal{H}_L=-c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}$$

$$\mathcal{H}_R=c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}$$

$$\boxed{\mathcal{H}_{\mathrm{K}}=v_{\mathrm{F}}\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}}$$

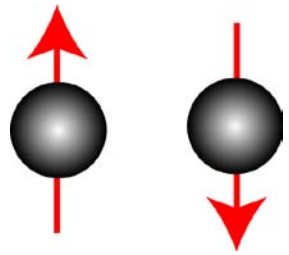
$$\boxed{\mathcal{H}_{K'}=v_{\mathrm{F}}\boldsymbol{\sigma}'\cdot\hat{\mathbf{p}}}\qquad\boldsymbol{\sigma}'=(-\sigma_x,\sigma_y)$$



Similar Hamiltonian for graphene with pseudo-spin

σ: operator for pseudo spin

Real spin and the magnetic field

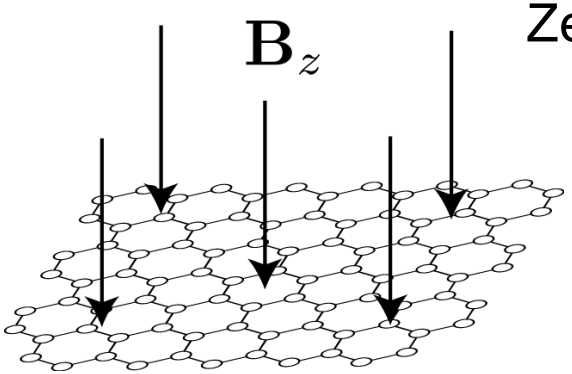


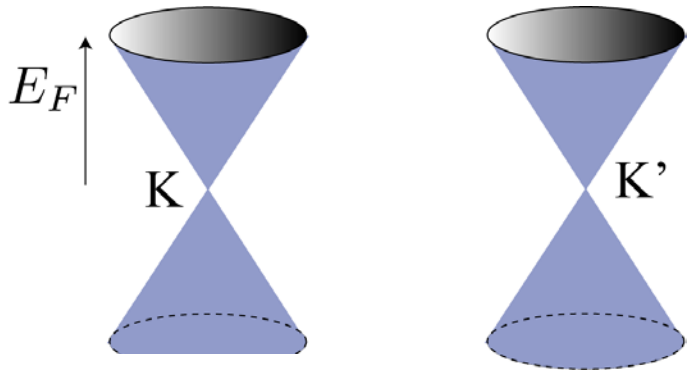
Vector field $\mathbf{B} = \nabla \times \mathbf{A}(\mathbf{r})$

$$\hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r})$$

$$\mathcal{H}_{\mathrm{e}} = \frac{(\hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r}))^2}{2m} - \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}(\mathbf{r}) + \cdots$$

Zeeman term





$$v_{\mathrm{F}}\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r})) \qquad v_{\mathrm{F}}\boldsymbol{\sigma}'\cdot(\hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r}))$$

Magnetic field does not polarize the pseudo spin.

$$+\mathbf{B}_z\sigma_z\begin{pmatrix}\Psi_{\mathrm{A}}\\ \Psi_{\mathrm{B}}\end{pmatrix}_{\mathrm{K}} \qquad -\mathbf{B}_z\sigma_z\begin{pmatrix}\Psi_{\mathrm{A}}\\ \Psi_{\mathrm{B}}\end{pmatrix}_{\mathrm{K}'}$$

Similar field A^q for pseudo spin

$$v_{\mathrm{F}}\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} + \mathbf{A}^{\mathrm{q}}(\mathbf{r})) \qquad v_{\mathrm{F}}\boldsymbol{\sigma}'\cdot(\hat{\mathbf{p}} - \mathbf{A}^{\mathrm{q}}(\mathbf{r}))$$

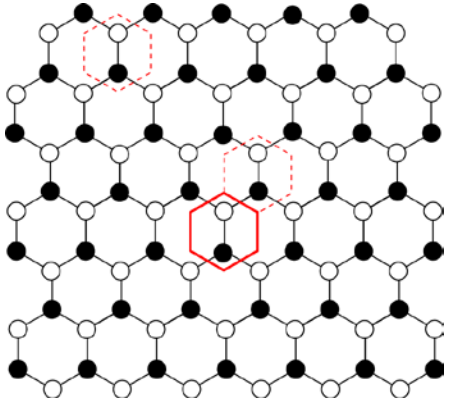
$$\mathbf{B}^{\mathrm{q}} = \nabla \times \mathbf{A}^{\mathrm{q}}(\mathbf{r})$$

$$+\mathbf{B}^{\mathrm{q}}_z\sigma_z\begin{pmatrix}\Psi_{\mathrm{A}}\\ \Psi_{\mathrm{B}}\end{pmatrix}_{\mathrm{K}} \qquad +\mathbf{B}^{\mathrm{q}}_z\sigma_z\begin{pmatrix}\Psi_{\mathrm{A}}\\ \Psi_{\mathrm{B}}\end{pmatrix}_{\mathrm{K}'}$$

Edge electronic states at the zigag edge of graphene

M. Fujita et al, J. Phys. Soc. Jpn. **65** (1996) 1920

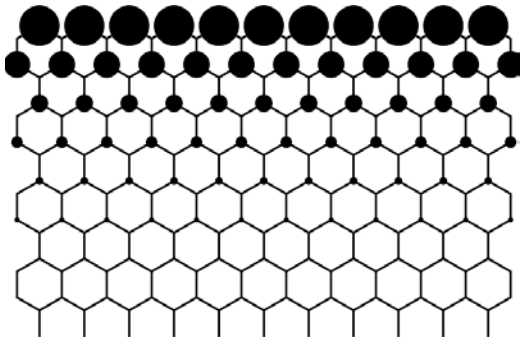
Delocalized states:



$$\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} \Psi_{\mathrm{A}}(\mathbf{k}) \\ \Psi_{\mathrm{B}}(\mathbf{k}) \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ e^{i\Theta(\mathbf{k})} \end{pmatrix}$$

Edge states:



● Amplitude of WF

Pseudo-spin polarized states

•W.F. has a value only either A or B site.

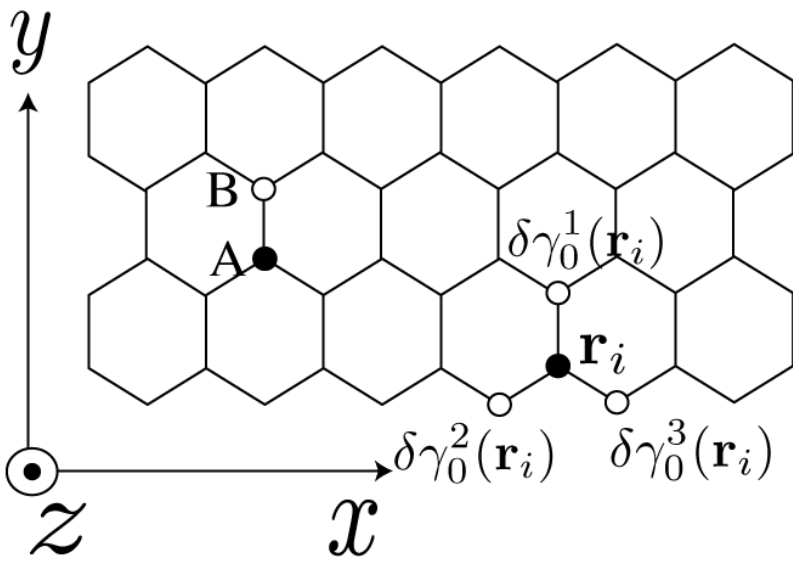
$$\Psi(\mathbf{r}) = \begin{pmatrix} \Psi_{\mathrm{A}}(\mathbf{r}) \\ 0 \end{pmatrix}$$

•Spacialy localized at zigzag edge

$$e^{-\frac{y}{\xi}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Vector potential for pseudo spin

K. Sasaki, R. Saito, *Prog. Theor. Phys. Suppl.* 176, 253 (2008)



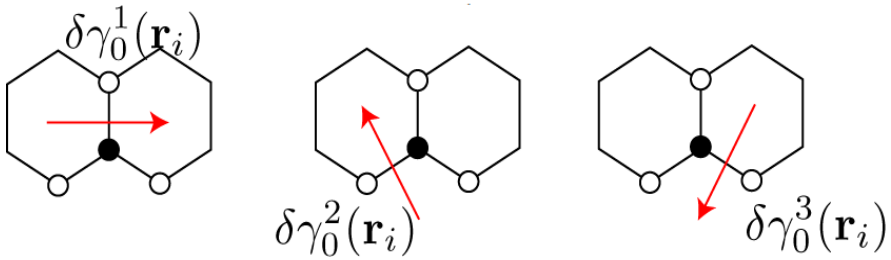
$$-\gamma_0 + \delta\gamma_0^a(\mathbf{r})$$

modification of nearest neighbor interaction

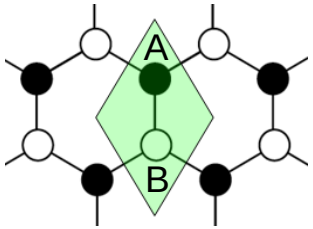
$$\mathcal{H}_{\mathrm{K}} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} + \mathbf{A}^{\mathrm{q}}(\mathbf{r}))$$

$$\mathcal{H}_{\mathrm{K}'} = v_{\mathrm{F}}\boldsymbol{\sigma}'\cdot(\hat{\mathbf{p}} - \mathbf{A}^{\mathrm{q}}(\mathbf{r}))$$

A^{q} is expressed by $\delta\gamma_0$



Why? modification of off-diagonal element with time reversal symmetry



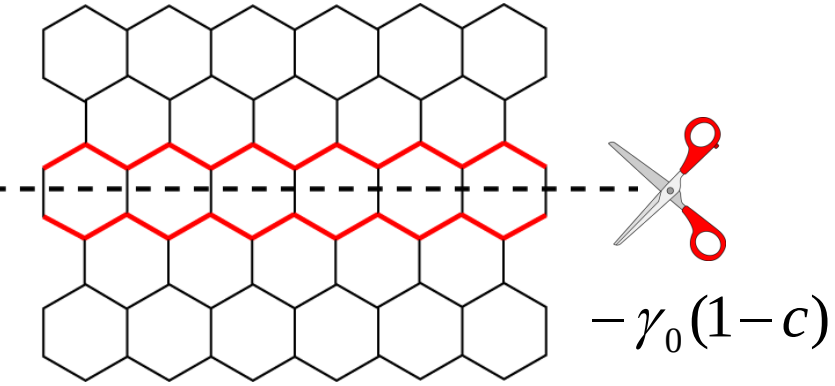
$$v_{\mathrm{F}}\begin{pmatrix} 0 & \hat{p}_x - i\hat{p}_y \\ \hat{p}_x + i\hat{p}_y & 0 \end{pmatrix}\begin{pmatrix} \psi_A(\mathbf{r}) \\ \psi_B(\mathbf{r}) \end{pmatrix} = E\begin{pmatrix} \psi_A(\mathbf{r}) \\ \psi_B(\mathbf{r}) \end{pmatrix}$$

$$\begin{pmatrix} 0 & A(\mathbf{r}) \\ A^*(\mathbf{r}) & 0 \end{pmatrix} \quad A(\mathbf{r}) = A_x(\mathbf{r}) - iA_y(\mathbf{r})$$

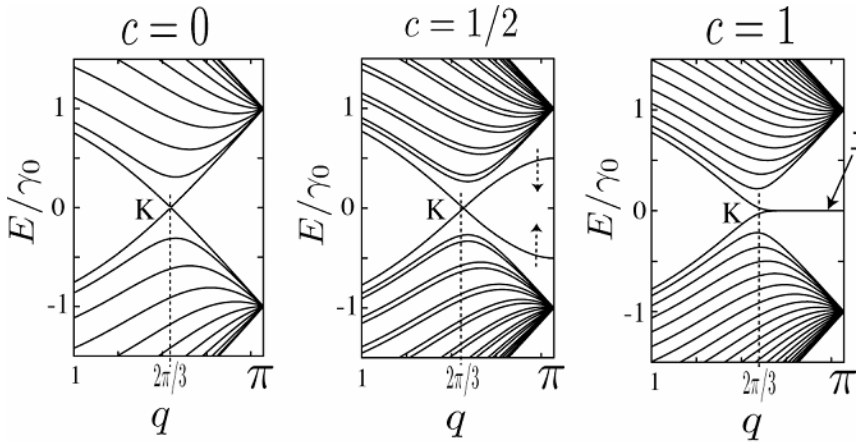
$$\mathcal{H}_{\mathrm{K}} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} + \mathbf{A}^{\mathrm{q}}(\mathbf{r}))$$

Analytic solution of zigzag edge states by A^q

K. Sasaki et al., J. Phys. Soc. Japan, **75,** 074713 (2006)



zigzag edge formation



tight binding results

A^q field results

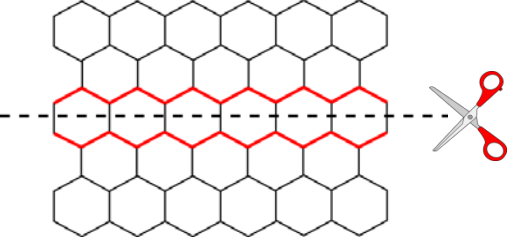
up: energy dispersion, down: localization length

$$\frac{E}{v_F} = \frac{\pm|p_x|}{\cosh\left(-\ln(1-c)\right)} + \mathcal{O}(ap_x^2/\hbar)$$

$$\frac{\hbar}{\xi} = p_x \tanh\left(-\ln(1-c)\right) + \mathcal{O}(ap_x^2/\hbar)$$

$$\frac{E}{v_F} = \frac{\pm|p_x|}{\cosh\left(\frac{1}{\hbar}\int_{-\xi_g}^{\xi_g} A_x(y)dy\right)}$$

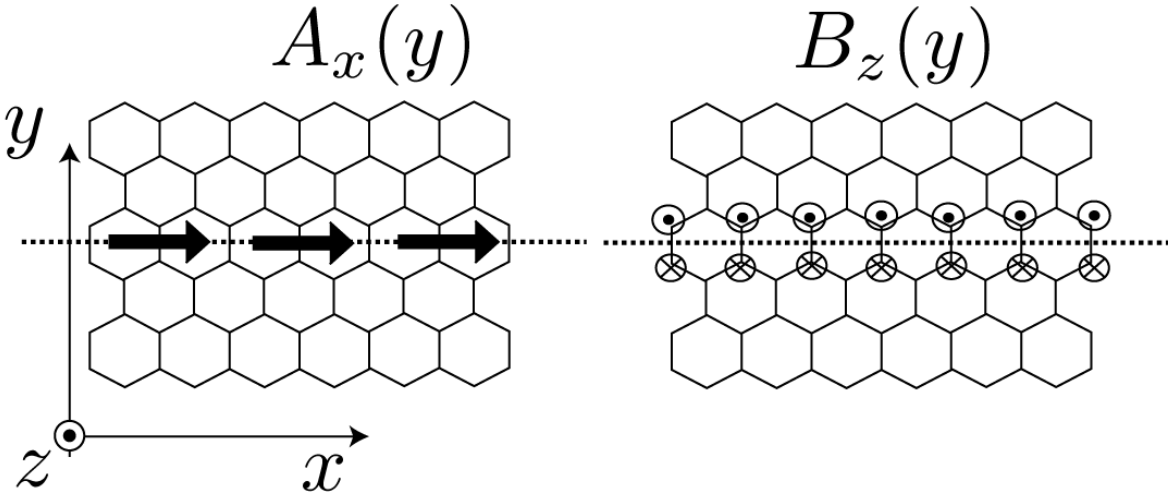
$$\frac{\hbar}{\xi} = p_x \tanh\left(\frac{1}{\hbar}\int_{-\xi_g}^{\xi_g} A_x(y)dy\right)$$

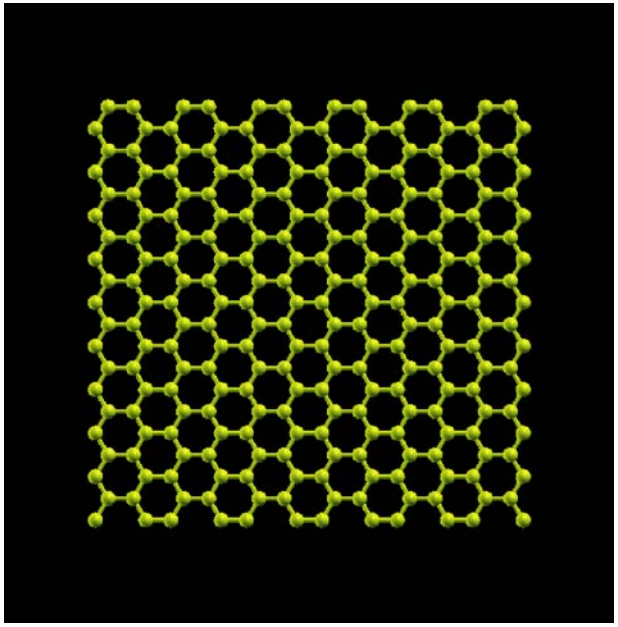


Zigzag edge vs Armchair edge

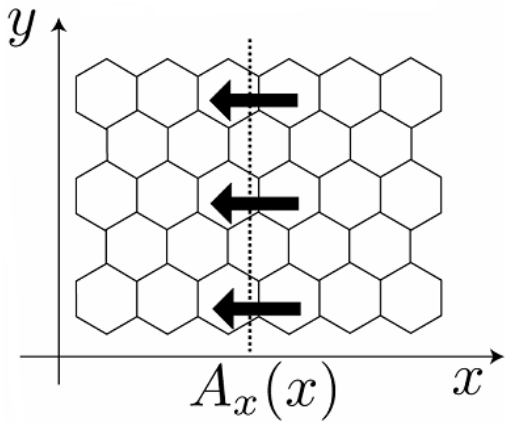
K. Sasaki et al., J. Phys. Soc. Japan, **75,** 074713 (2006)

Zigzag edge





Armchair edge

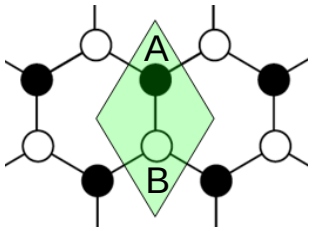


$$B_z = 0$$

$$B_z(\mathbf{r}) = \frac{\partial A_y(\mathbf{r})}{\partial x} - \frac{\partial A_x(\mathbf{r})}{\partial y}$$

No pseudo-spin polarization → no edge states

Useful for considering edge states for any edge



Direction of Pseudo-Spin

Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

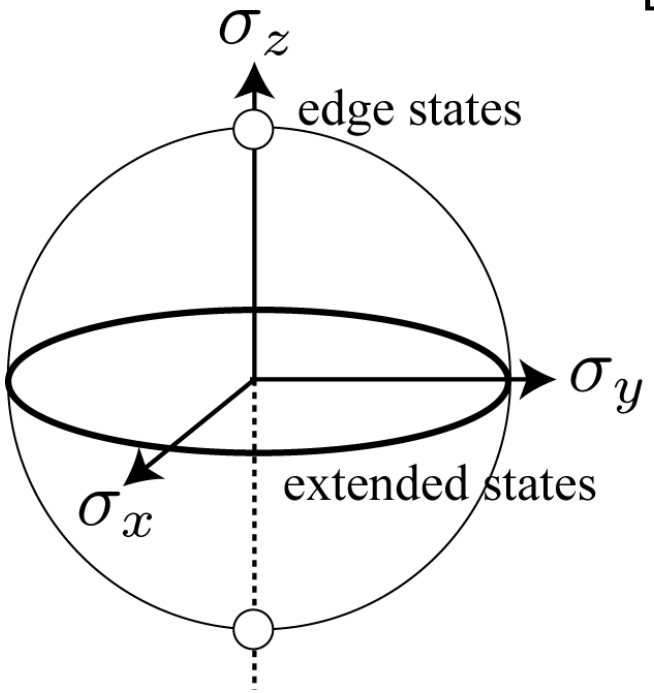
Extended states

$$\Psi(\mathbf{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{+i\Theta(\mathbf{k})} \end{pmatrix}$$

$$\langle \sigma_x \rangle = \cos\Theta(\mathbf{k})$$

$$\langle \sigma_y \rangle = \sin\Theta(\mathbf{k})$$

$$\langle \sigma_z \rangle = 0$$



Edge states

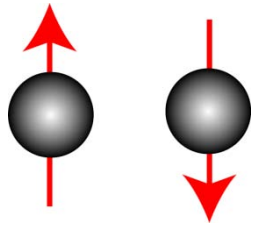
$$\Psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\langle \sigma_x \rangle = 0$$

$$\langle \sigma_y \rangle = 0$$

$$\langle \sigma_z \rangle = 1$$

$$\langle \sigma_z \rangle = \frac{1}{2} \begin{pmatrix} 1 & e^{-i\Theta(k)} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ e^{+i\Theta(k)} \end{pmatrix} = 0$$



$\langle \sigma_z \rangle$

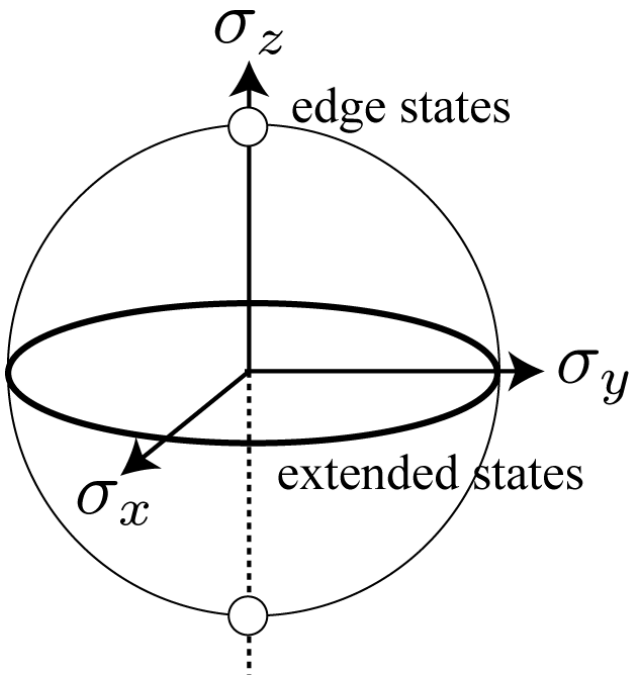
Parity anomaly in graphene – origin of the mass –

K. Sasaki, R. Saito, J. Phys. Soc. Japan, 77, 054703 (2008)

Weyl equation (periodic system)

$$\mathcal{H}_{\mathrm{K}}^{\mathrm{periodic}} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot\mathbf{p}$$

$$\boldsymbol{\sigma}\cdot\mathbf{p} = \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$



Weyl equation (finite system)

Zigzag edge

$$\mathcal{H}_{\mathrm{K}}^{\mathrm{finite}} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot\left(\mathbf{p} + \mathbf{A}^{\mathrm{q}}(\mathbf{r})\right)$$

$$B_z^{\mathrm{q}}(\mathbf{r}) = \nabla\times\mathbf{A}^{\mathrm{q}}(\mathbf{r})$$

$$v_{\mathrm{F}}\boldsymbol{\sigma}\cdot\left(\mathbf{p} + \mathbf{A}^{\mathrm{q}}(\mathbf{r})\right) + m_s\sigma_z$$

$$\langle n_s(\mathbf{r})\rangle = \frac{1}{2}\frac{B_z^{\mathrm{q}}(\mathbf{r})}{\Phi_0}\mathrm{sign}(m_s)$$

Broken A and B symmetry
Partial polarization of pseudo-spin
Occurrence of the mass

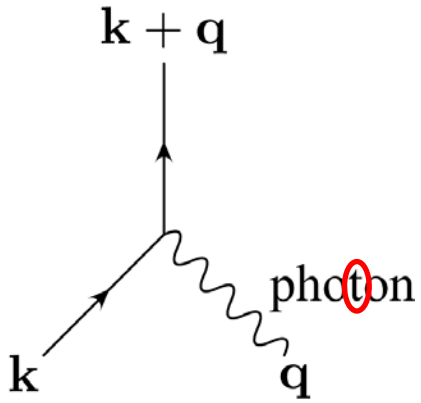
Most simple realization of Parity anomaly

1. Deformation-induce magnetic field
2. Coulomb-induce mass term

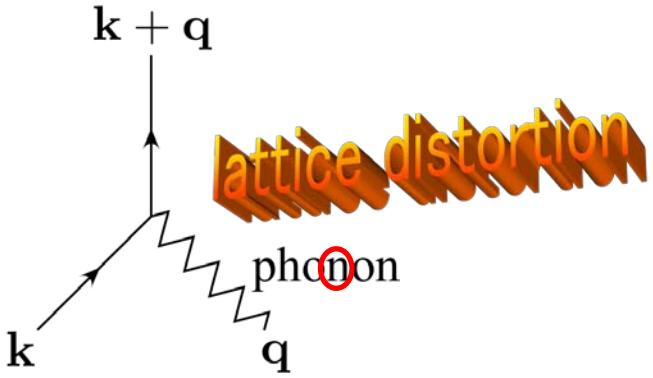
Electron-phonon interaction is expressed by A^q

K. Sasaki, R. Saito, G. Dresselhaus, M. S. Dresselhaus, H. Farhat, J. Kong, Phys. Rev. B, 77, 245441 (2008)

Electron-photon interaction



Electron-phonon interaction



K point $\quad \hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r})$ $\qquad \hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} + \mathbf{A}^q(\mathbf{r})$

K'point $\quad \hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r})$ $\qquad \hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} - \mathbf{A}^q(\mathbf{r})$

Broken time-reversal symmetry

Time-reversal symmetry over the k space

$$\mathbf{B} = \nabla \times \mathbf{A}(\mathbf{r})$$

$$\mathbf{B}^q = \nabla \times \mathbf{A}^q(\mathbf{r})$$

Electro-chemical doping and Raman spectrosocpy of single wall carbon nanotubes

Farhat *et al*., *Phys. Rev. Lett.*, 99 145506(2007)

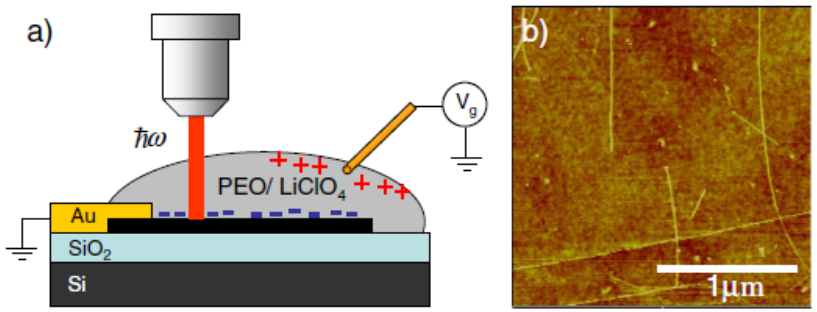
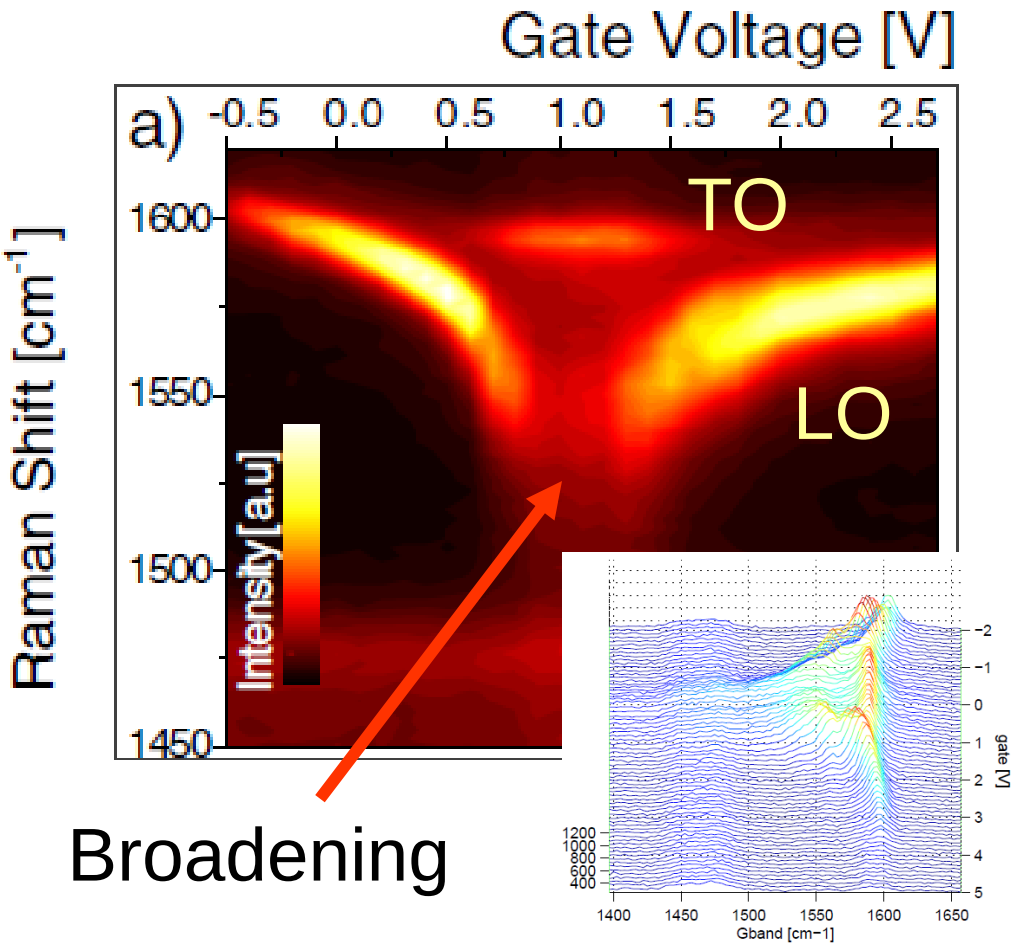


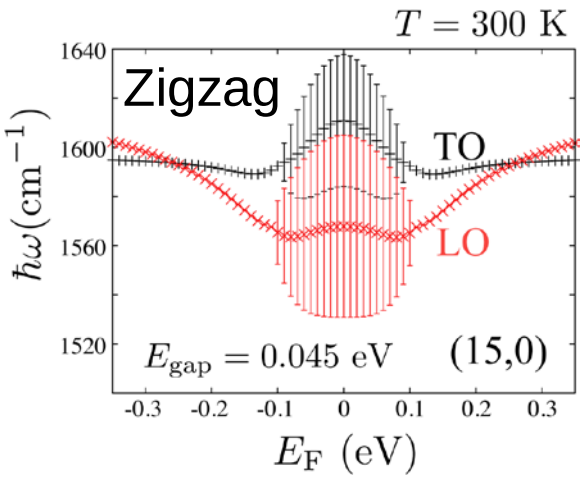
FIG. 1 (color online). (a) Schematic diagram of the experimental setup. The excitation laser shines through the PEO/$LiClO_4$ polymer electrolyte. (b) An AFM image indicating that the nanotubes are spaced out and are typically isolated from one another.

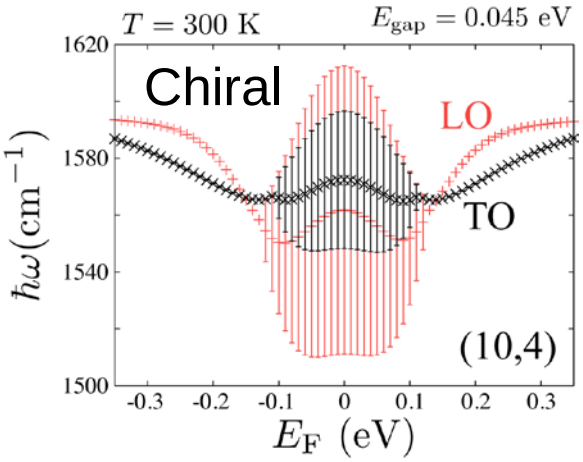
- isolated metallic SWNT
- E_F dependent
- upshift of TO?

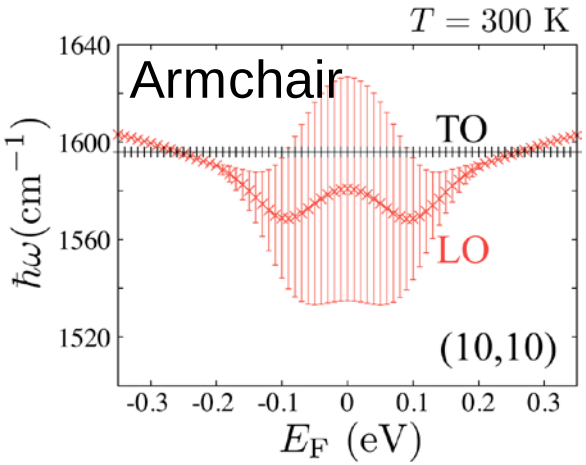


Chiral angle dependence of KA

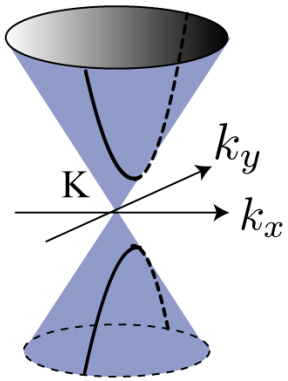
K. Sasaki, R. Saito, et al. Phys. Rev. B, 77, 245441 (2008)

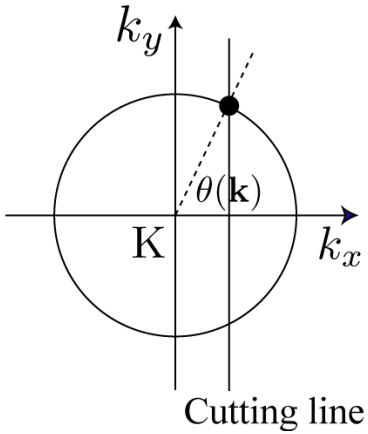






Why TO becomes hard for zigzag NT?





Θ dependent el-ph interaction

LO: $\langle \mathrm{eh}(\mathbf{k})|\mathcal{H}_{\mathrm{ep}}|\omega_l\rangle = -igu\sin\theta(\mathbf{k})$

TO: $\langle \mathrm{eh}(\mathbf{k})|\mathcal{H}_{\mathrm{ep}}|\omega_t\rangle = -igu\cos\theta(\mathbf{k})$

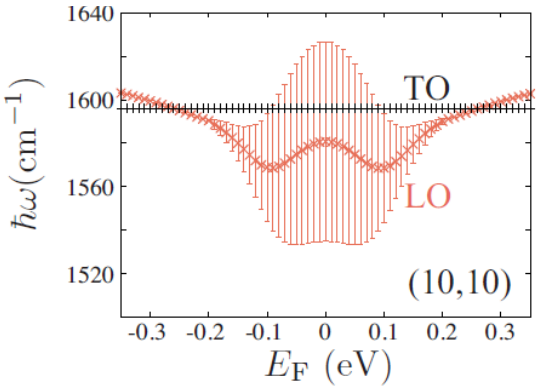
$$v_{\mathrm{F}}(A_x(\mathbf{r}), A_y(\mathbf{r})) = g(u_y(\mathbf{r}), -u_x(\mathbf{r}))$$

K. Ishikawa and T. Ando, J. Phys. Soc. Jpn. **75**, 84713 (2006).
T. Ando, J. Phys. Soc. Jpn. **77**, 14707 (2008).

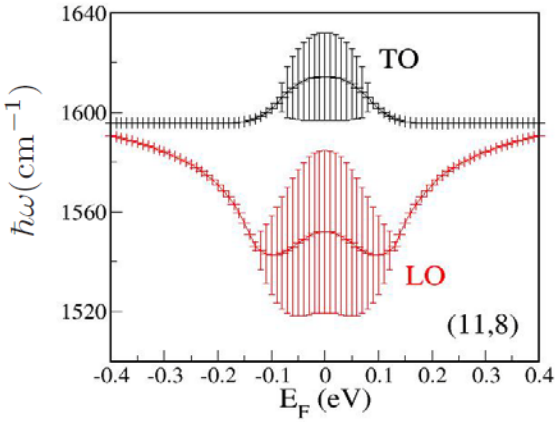
Gate voltage dependence of G band Raman spectra

J. S. Park, *et al.* unpublished

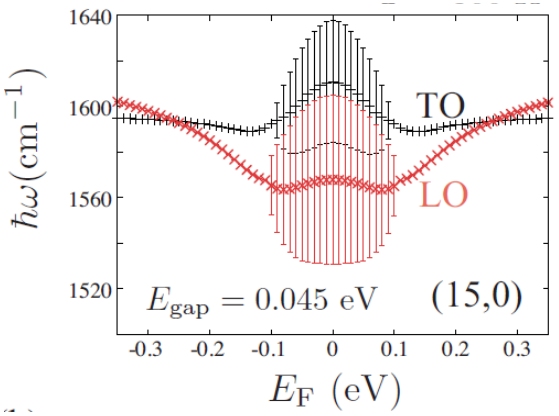
Armchair SWNT



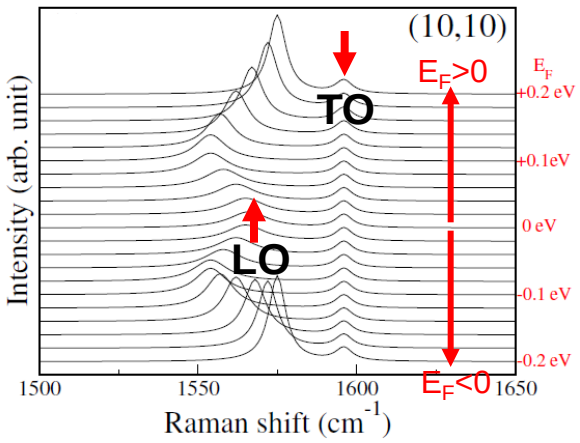
Chiral SWNT

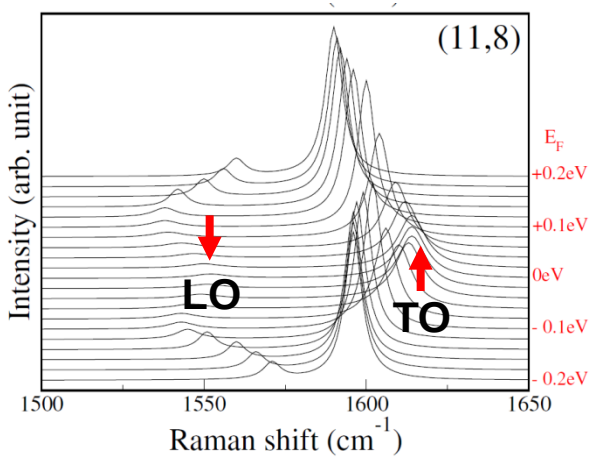


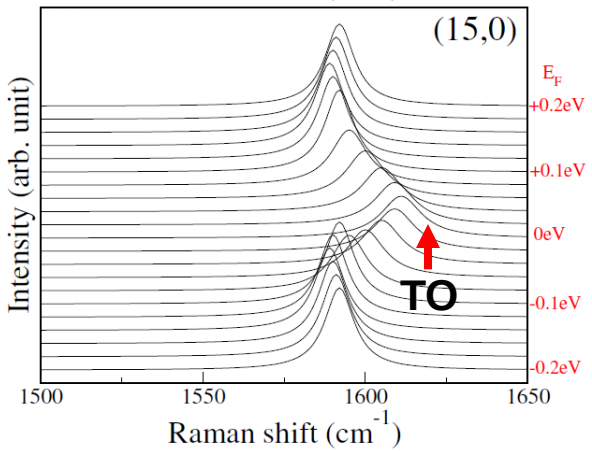
Zigzag SWNT



K. Sasaki, *et al.* Phys. Rev. B 77, 245441 (2008)







For LO mode of zigzag tube,
No Electron-phonon int.

Edge states superconductivity of graphene

K. Sasaki, et al., *J. Phys. Soc. Japan*, 76, 033702, (2007)

$$T_c > 10\mathrm{K}\ !?$$

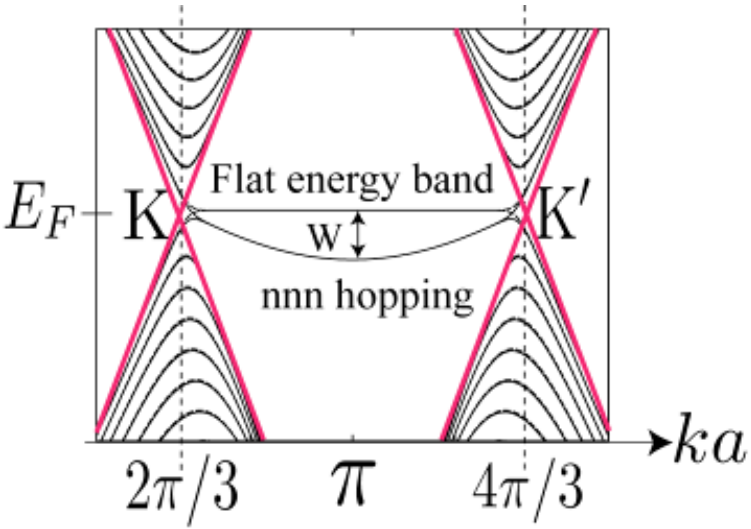
Tang *et al.*, Science **292** (01) for SWNT (0.4nm diameter)
Takesue *et al.*, PRL **96** (06) for MWNT (10nm diameter)

Two problems

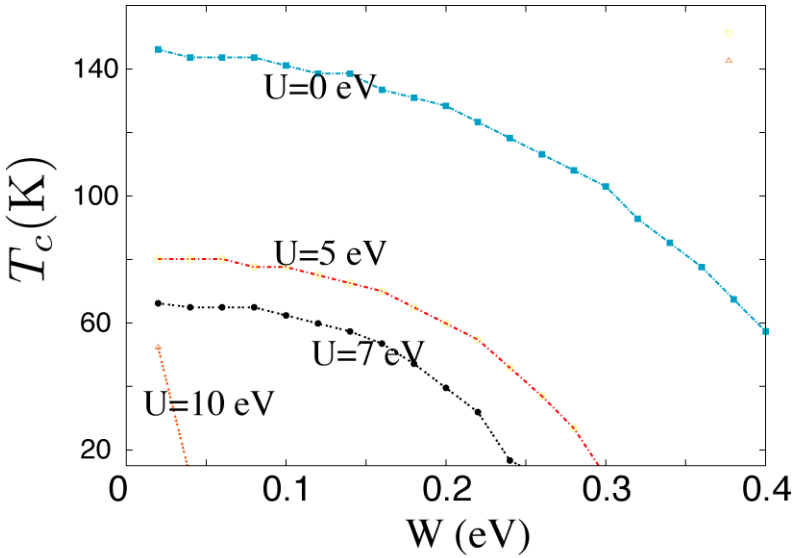
1. no $D(E_F)$
2. suppression of el-ph interaction

U : repulsive Coulomb interaction

Edge states could overcome the problems.



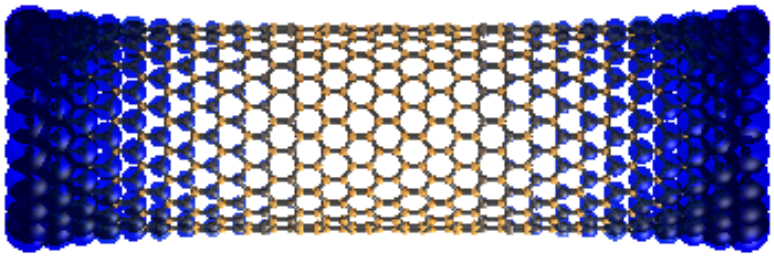
Eliashberg equation



Energy bandwidth of edge states

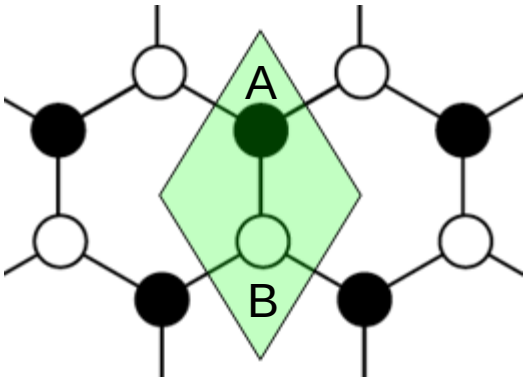
$$W = \gamma_n$$

K. Sasaki et al., Appl. Phys. Lett., 88, 113110 (2006)



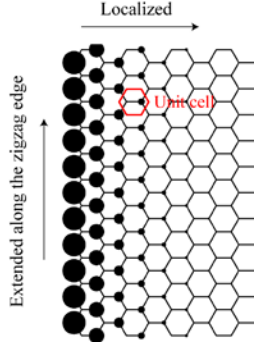
Summary

Pseudo Spin and A^q

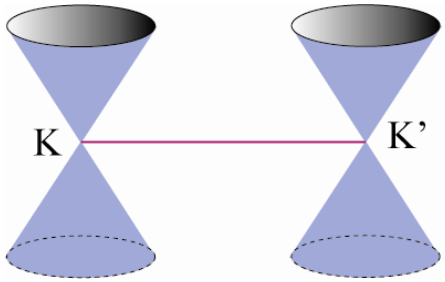


Edge states: polarized pseudo spin

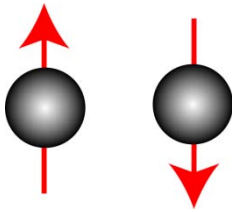
$$\begin{pmatrix}\Psi_A\\ \Psi_B\end{pmatrix} = e^{-\frac{x}{\xi}}\begin{pmatrix}1\\ 0\end{pmatrix}$$



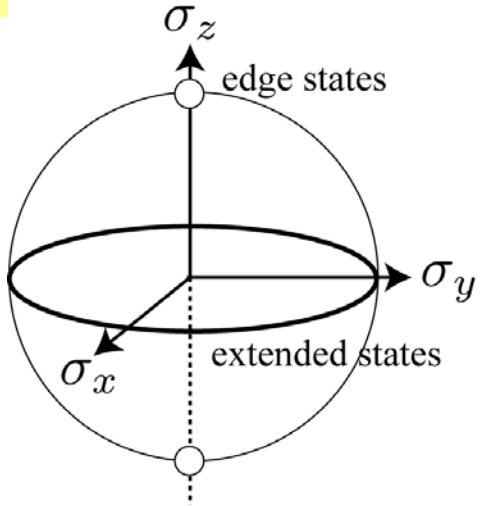
Strong electron-phonon interaction
superconductivity

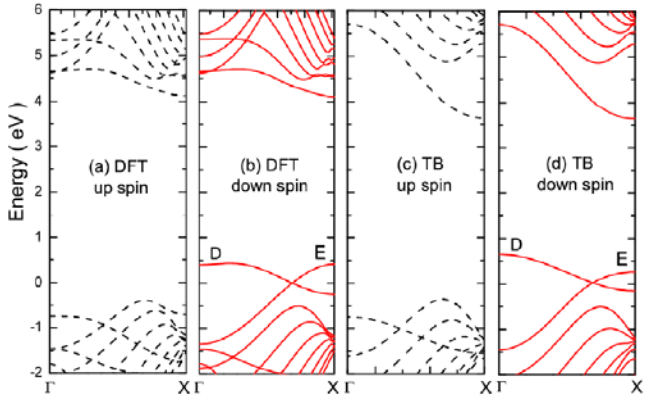


similarity to real spin



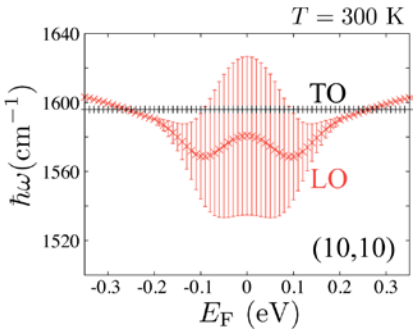
$\langle \sigma_z \rangle$: Edge states parameter





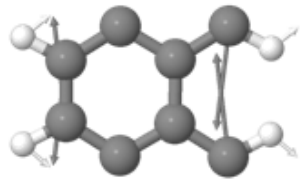
4-AGNR-4H 1535 cm^{-1}

Application of A^q to el-ph interaction



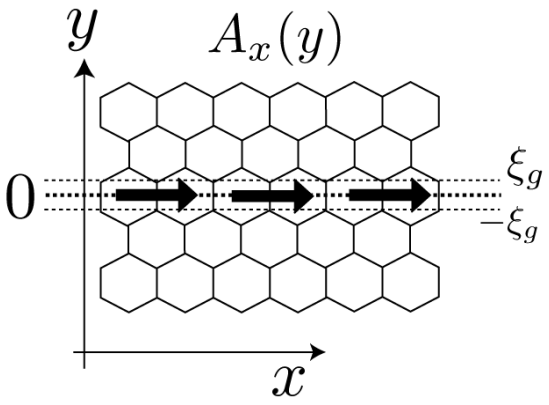
$$v_F\boldsymbol{\sigma}\cdot\left(\mathbf{p}+\mathbf{A}^q(\mathbf{r})\right)+m_s\sigma_z$$

$$\langle n_s(\mathbf{r})\rangle = \frac{1}{2}\frac{B_z^q(\mathbf{r})}{\Phi_0}\mathrm{sign}(m_s)$$



Thank you.

$$v_{\mathrm{F}}\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}}+\mathbf{A}(\mathbf{r}))\begin{pmatrix}\psi_A(\mathbf{r})\\ \psi_B(\mathbf{r})\end{pmatrix}=E\begin{pmatrix}\psi_A(\mathbf{r})\\ \psi_B(\mathbf{r})\end{pmatrix}$$



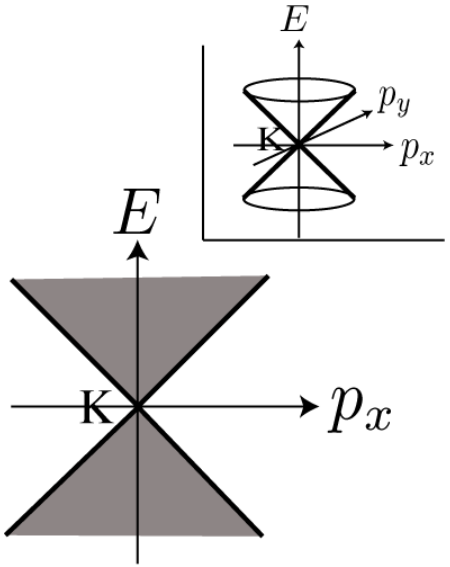
局在解 $$\begin{pmatrix}\psi_A(\mathbf{r})\\ \psi_B(\mathbf{r})\end{pmatrix}=Ne^{i\frac{p_x x}{\hbar}}e^{-\frac{|y|}{\xi}}\begin{pmatrix}e^{+g(y)}\\ e^{-g(y)}\end{pmatrix}$$

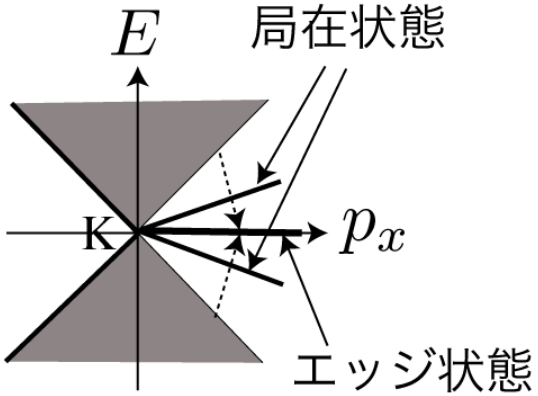
$$\frac{E}{v_F}=\frac{\pm|p_x|}{\cosh\left(\frac{1}{\hbar}\int_{-\xi_g}^{\xi_g}A_x(y)dy\right)}$$

$$\frac{\hbar}{\xi}=p_x\tanh\left(\frac{1}{\hbar}\int_{-\xi_g}^{\xi_g}A_x(y)dy\right)$$

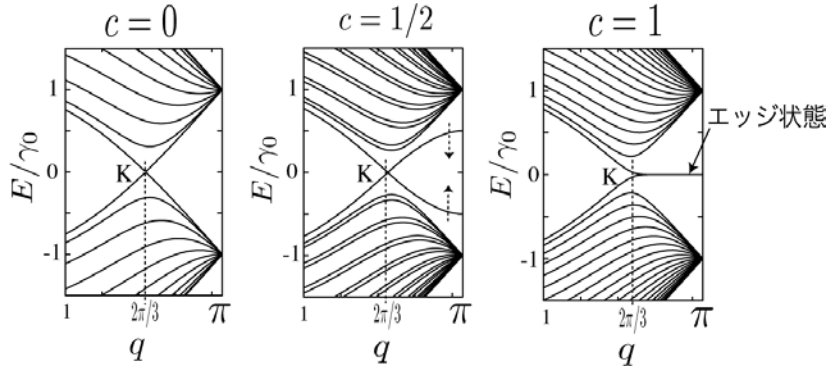
$$g(y)=\begin{cases}+\frac{1}{2}\int_{-\xi_g}^{\xi_g}A_x(y)dy & (y\le-\xi_g)\\ -\frac{1}{2}\int_{-\xi_g}^{\xi_g}A_x(y)dy & (y\ge-\xi_g)\end{cases}$$

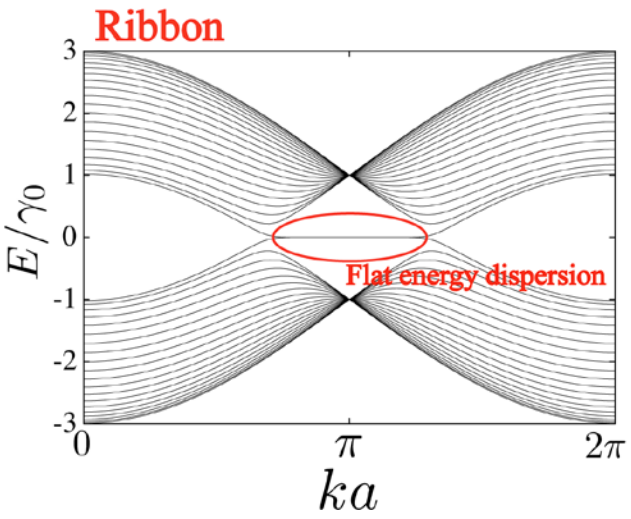
Sasaki *et al.*, JPSJ**75** (2006)

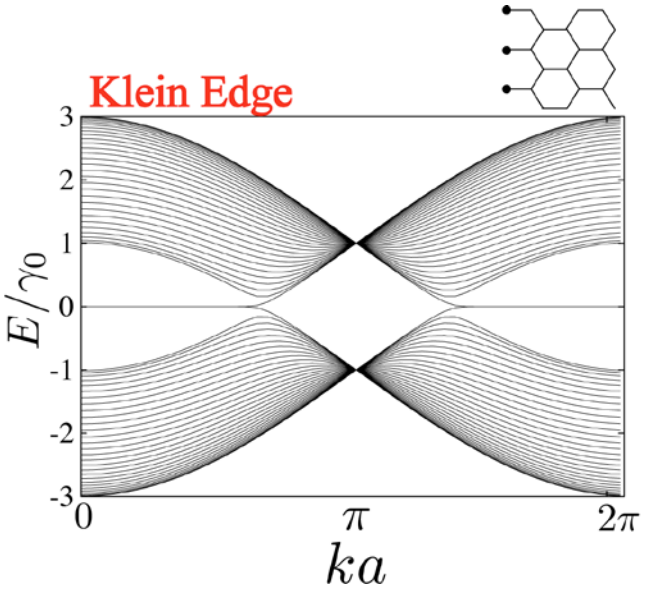


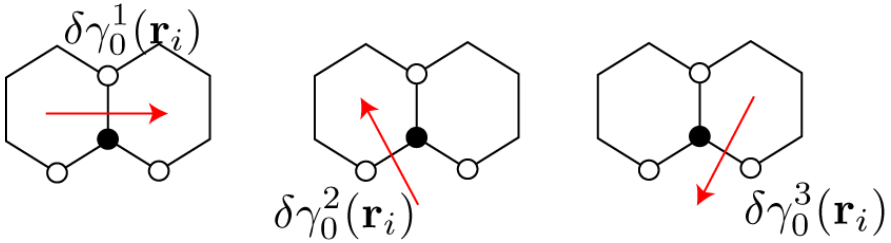


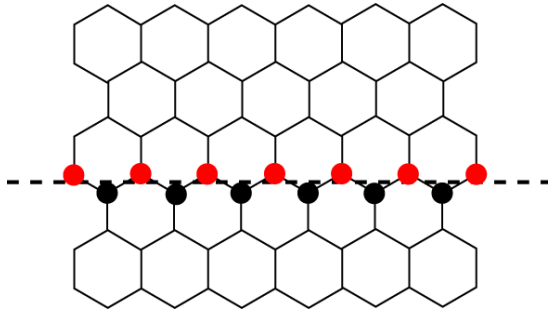
- **ほとんどゼロエネルギー状態**
- **局在長がエッジに沿った方向の波数に依存**











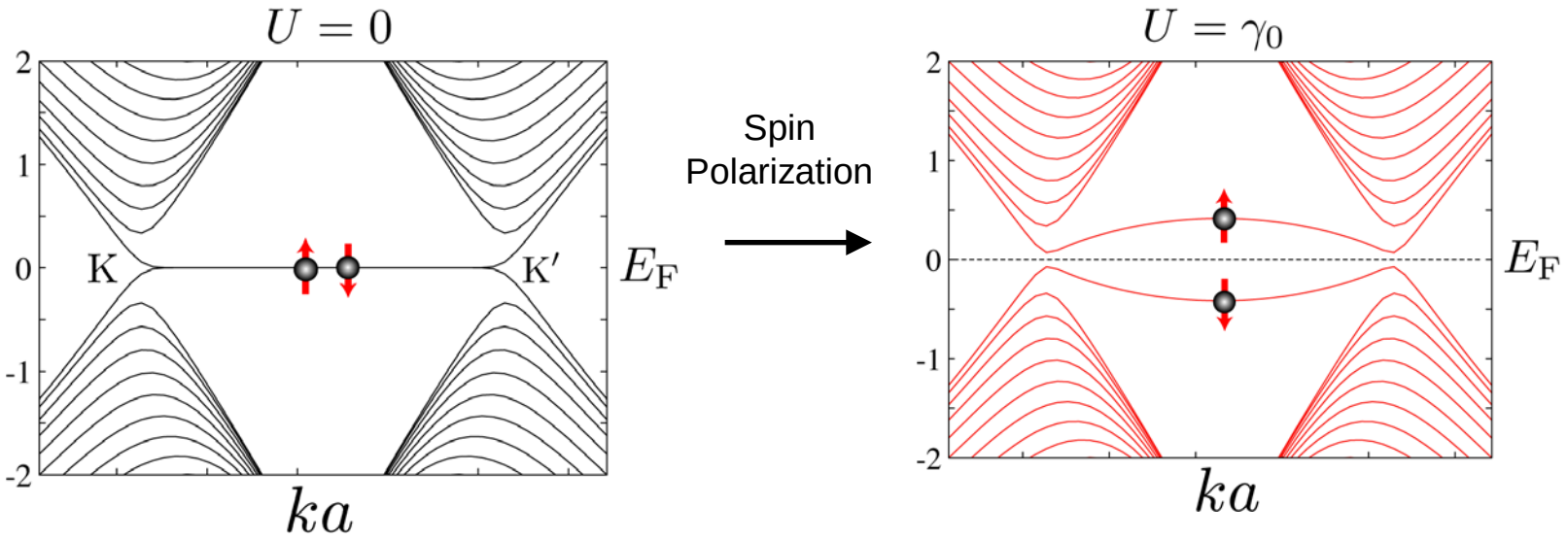
$$v_{\mathrm{F}} A_x(\mathbf{r}) = \delta\gamma_0^1(\mathbf{r}) - \frac{1}{2}\left(\delta\gamma_0^2(\mathbf{r}) + \delta\gamma_0^3(\mathbf{r})\right)$$

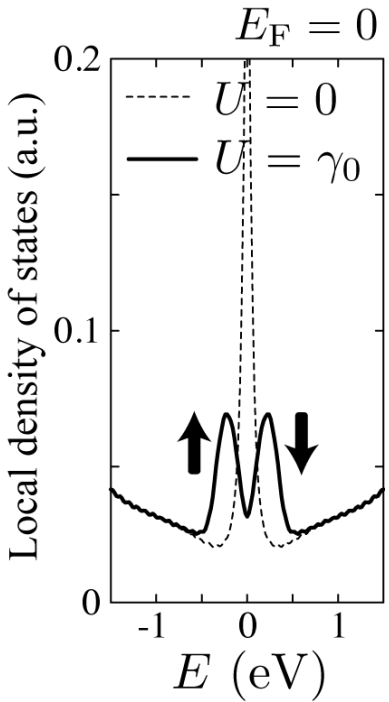
$$v_{\mathrm{F}} A_y(\mathbf{r}) = \frac{\sqrt{3}}{2}\left(\delta\gamma_0^2(\mathbf{r}) - \delta\gamma_0^3(\mathbf{r})\right)$$

$$\frac{\hbar}{\xi} = p_x \tanh\left(\frac{1}{\hbar}\int_{-\xi_g}^{\xi_g} A_x(y)dy\right)$$

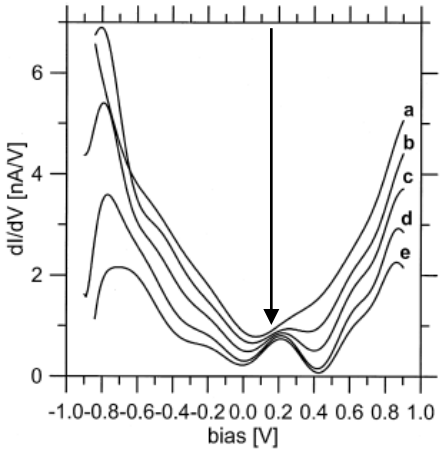
Single peak or double peaks?

$$\mathcal{H}_{\rm int} = U \sum_{\mathbf{r}} n_\uparrow(\mathbf{r}) n_\downarrow(\mathbf{r})$$

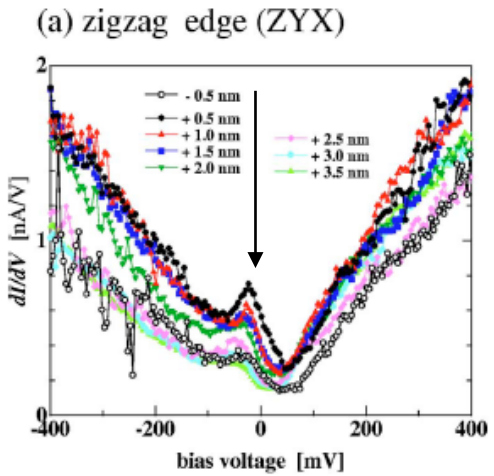




STS experiments for a step edge in graphite



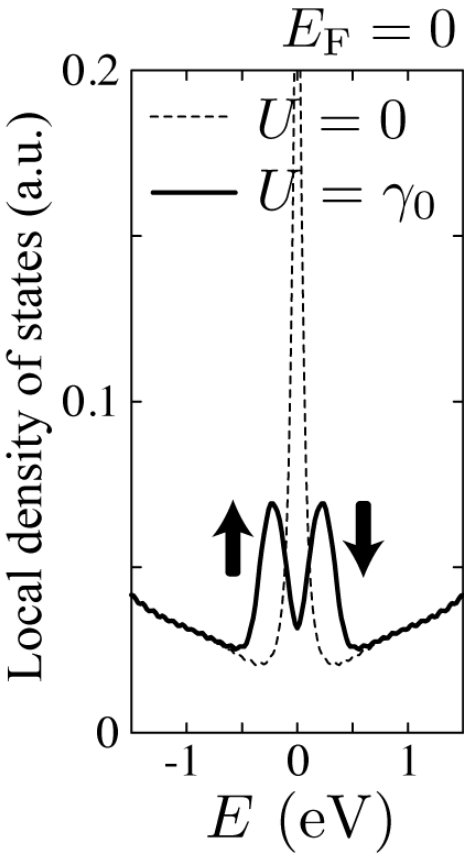
Klusek *et al.*, Appl. Surf. Sci. **161** (2000)

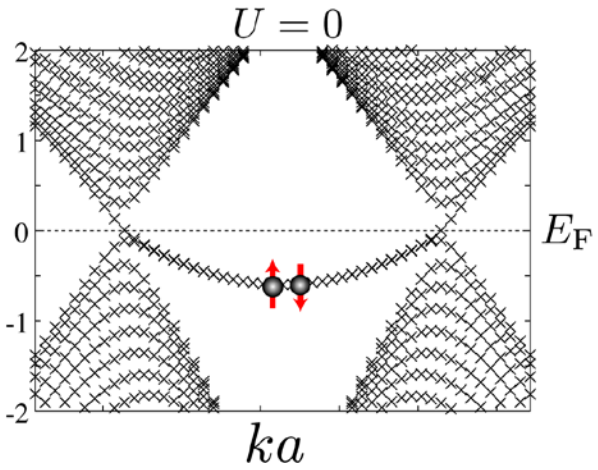


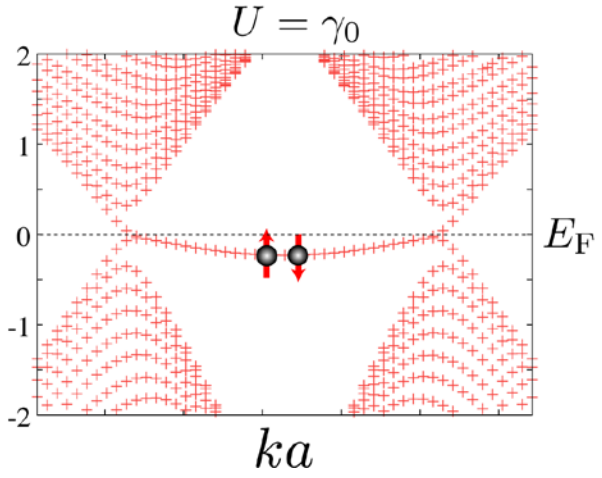
Niimi *et al.*, Appl. Surf. Sci. **241** (2005)

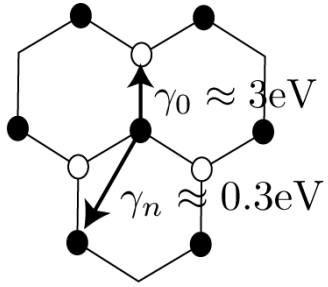
Kobayashi *et al.*, PRB **71** (2005)

$\gamma_n = 0.6$ eV

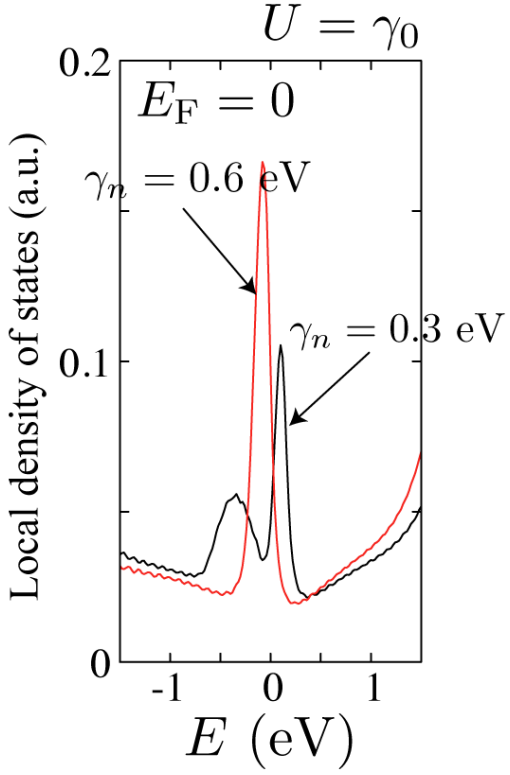




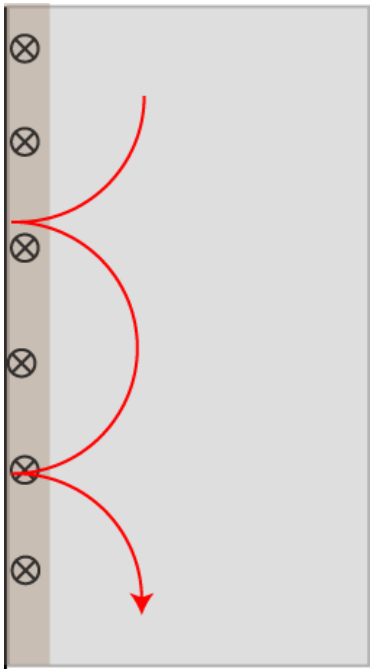


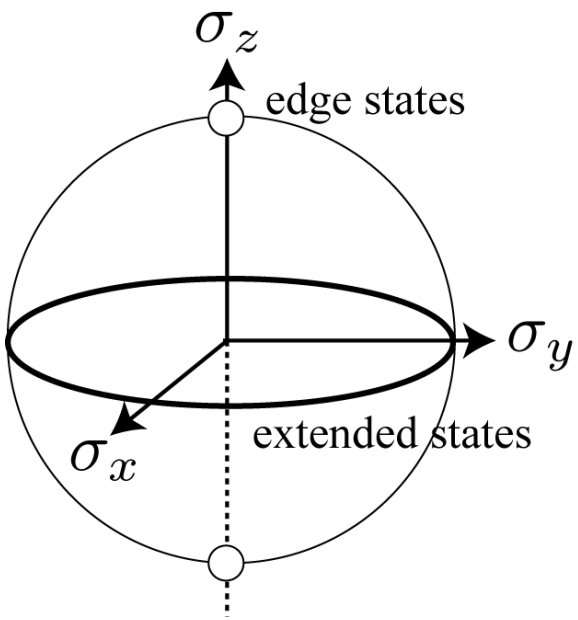


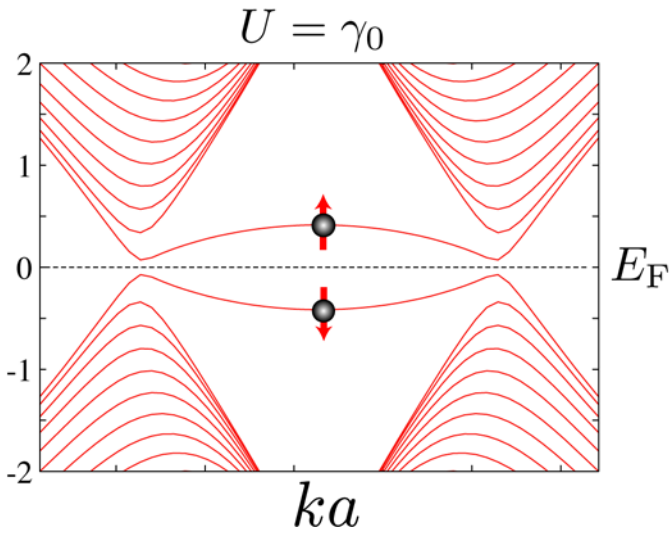
next nearest-neighbor (nnn)



Sasaki *et al.*, arXiv:0801.4170
to appear in J. Phys. Soc. Jpn. (2008)







Mass from Coulomb interaction

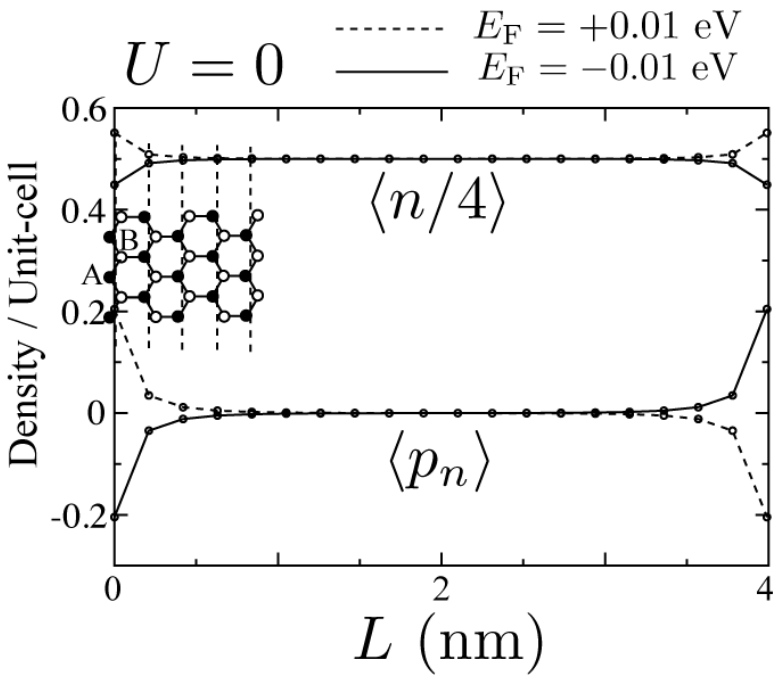
$$v_F \boldsymbol{\sigma} \cdot (\mathbf{p} + \mathbf{A}^q(\mathbf{r})) + m_s \sigma_z$$

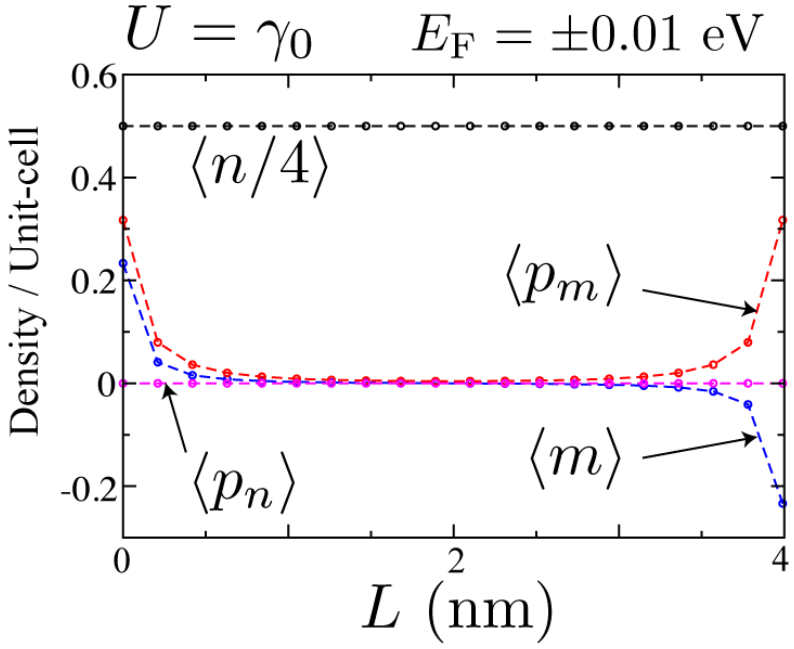
$$\frac{U}{4}(p_n - p_m)\sigma_z = m_\uparrow \sigma_z$$

$$\frac{U}{4}(p_n + p_m)\sigma_z = m_\downarrow \sigma_z$$

$$\langle n_s(\mathbf{r}) \rangle = \frac{1}{2} \frac{B_z^q(\mathbf{r})}{\Phi_0} \mathrm{sign}(m_s)$$

Mean field approximation





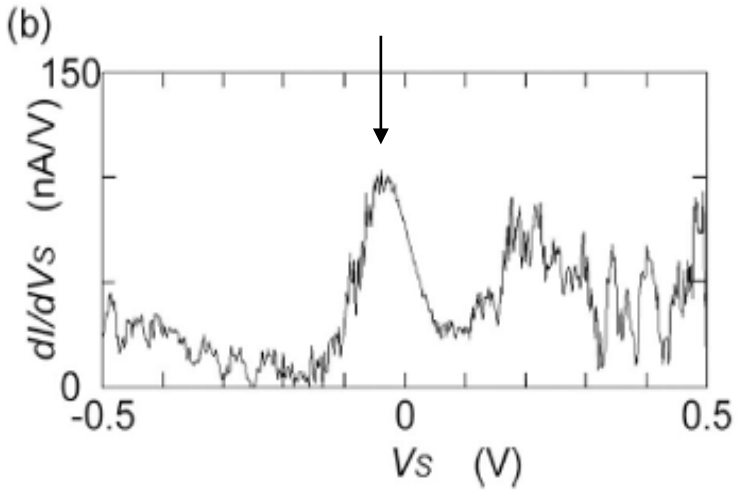
$$\mathcal{H}_{\rm int} = \frac{U}{8} \sum_{\mathbf{R}_u} (n^2 - m^2 + p_n^2 - p_m^2)$$

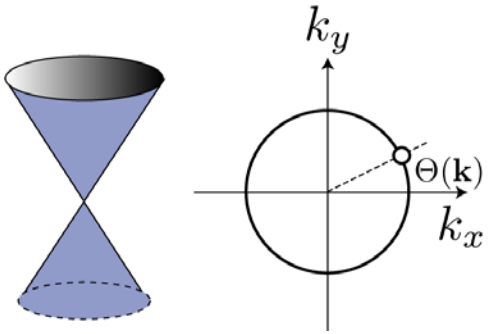
Equal densities at A and B atoms

$$p_n = n_{\rm A} - n_{\rm B}$$

Pseudo-spin polarization disappears, and Real-spin is polarized

$$\mathcal{H}_{\rm int} = \frac{U}{8} \sum_{\mathbf{R}_u} (n^2 - m^2 + p_n^2 - p_m^2)$$

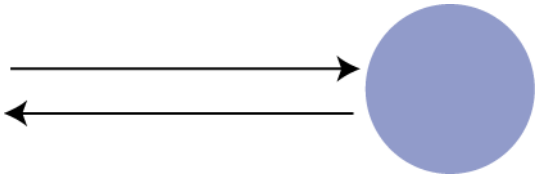




後方散乱の抑制

不純物による散乱

$$\Psi(k_x) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$



$$\langle -k_x | \mathcal{H}_{\rm imp} | k_x \rangle$$

$$\Psi(\mathbf{k}) = \begin{pmatrix} 1 \\ e^{+i\Theta(\mathbf{k})} \end{pmatrix}$$

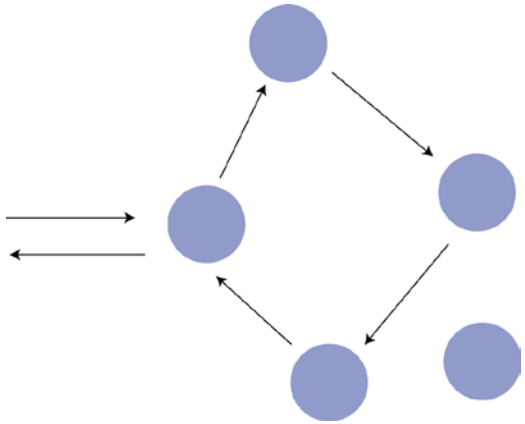
$$\Psi(-k_x) = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

波数に依存した相対位相

$$(1,-1)\begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = 0$$

多重散乱でも後方散乱が抑制

Nakanishi *et al.*, JPSJ**67**, 2857(98)



２成分間の干渉効果

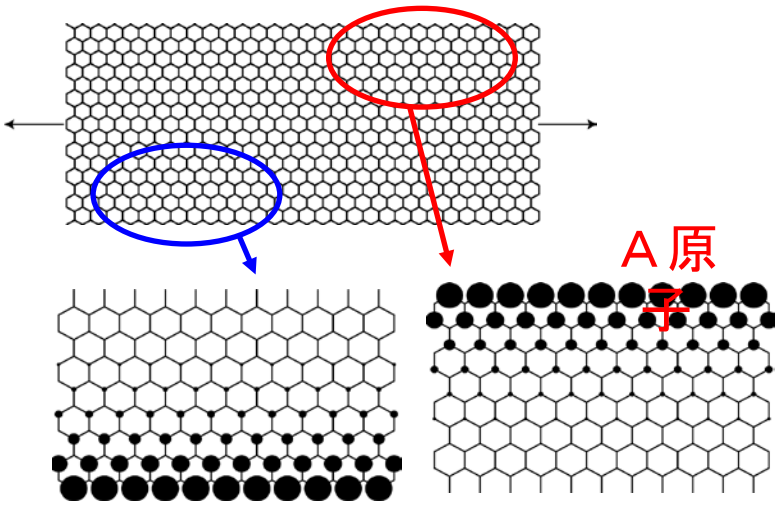
Suzuura and Ando, PRB**65**, 235412(02)

エッジ状態

$$(1,0)\begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = V$$

二成分間の相対位相や大きさの比（擬スピン）が物性に関係

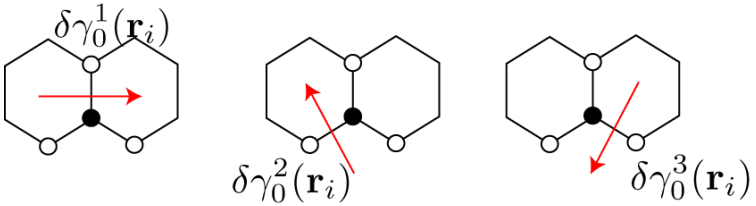
$$B_z^{\mathrm{q}}(\mathbf{r}) = \frac{\partial A_y(\mathbf{r})}{\partial x} - \frac{\partial A_x(\mathbf{r})}{\partial y}$$

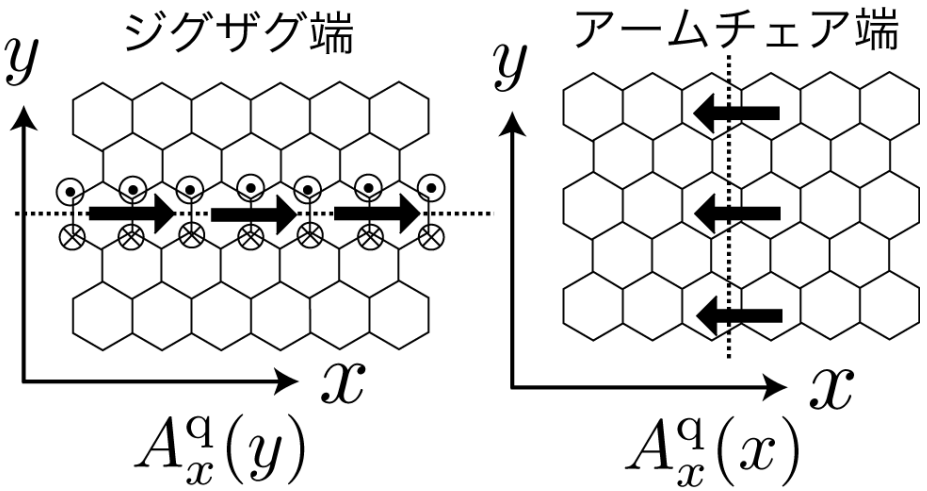


$$\mathcal{H}_{\mathrm{K}} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} + \mathbf{A}^{\mathrm{q}}(\mathbf{r}))$$

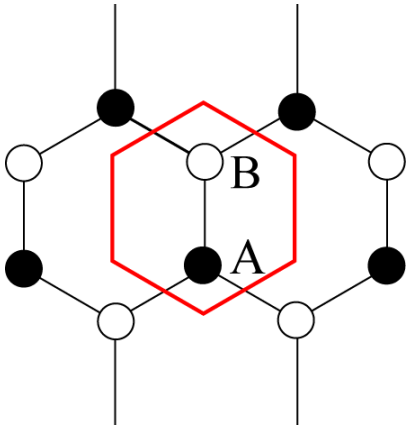
エッジ状態の性質をすべて再現する。

Sasaki *et al.*, JPSJ**75** (2006)





グラフェンの擬スピンとは何か



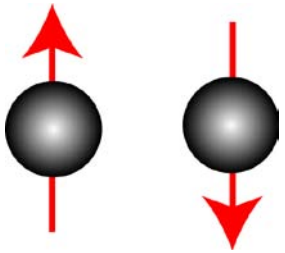
$$\mathcal{H}_{\mathrm{K}} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}$$

$$\mathcal{H}_{\mathrm{K}'} = v_{\mathrm{F}}\boldsymbol{\sigma}'\cdot\hat{\mathbf{p}}$$

実スピン

$$E\begin{pmatrix}\Psi_L\\ \Psi_R\end{pmatrix} = \begin{pmatrix}-c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}} & mc^2 I\\ mc^2 I & c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}\end{pmatrix}\begin{pmatrix}\Psi_L\\ \Psi_R\end{pmatrix}$$

ディラック方程式と電磁場

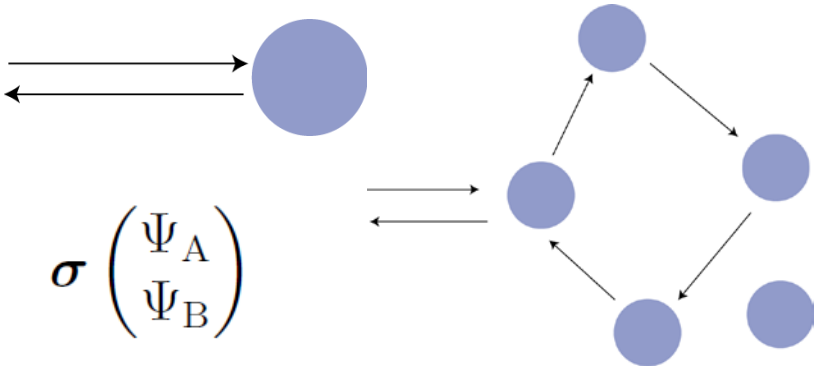


$$\hat{\mathbf{p}} \to \hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r})$$

$$\mathbf{B} = \nabla\times\mathbf{A}(\mathbf{r})$$

まとめ

二成分間の相対位相



$$\boldsymbol{\sigma}\begin{pmatrix}\Psi_{\mathrm{A}}\\ \Psi_{\mathrm{B}}\end{pmatrix}$$

後方散乱の抑制

エッジ状態

$$(1,0)\begin{pmatrix}V & 0\\ 0 & V\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = V$$

$$\mathcal{H}_{\mathrm{K}} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} + \mathbf{A}^{\mathrm{q}}(\mathbf{r}))$$

$$\mathcal{H}_{\mathrm{K}'} = v_{\mathrm{F}}\boldsymbol{\sigma}'\cdot(\hat{\mathbf{p}} - \mathbf{A}^{\mathrm{q}}(\mathbf{r}))$$

$$\mathbf{B}^{\mathrm{q}} = \nabla\times\mathbf{A}^{\mathrm{q}}(\mathbf{r})$$

擬スピンをそろえる場

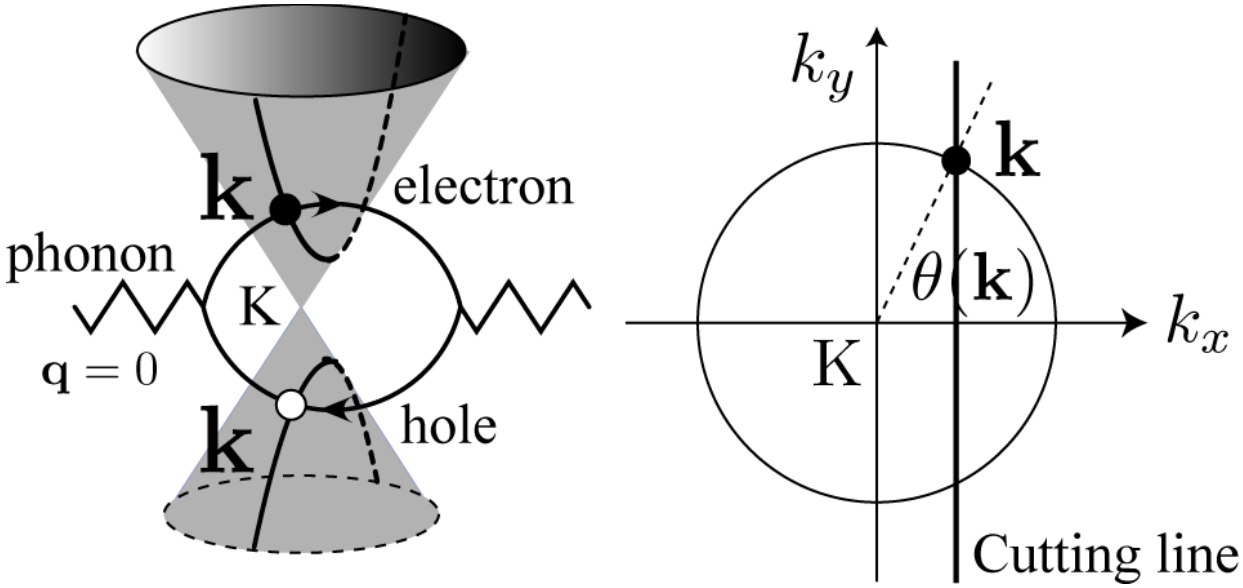
$$\mathcal{H}^{\mathrm{K}} = v_{\mathrm{F}}\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} + \mathbf{A}^{\mathrm{q}}(\mathbf{r})) + \frac{g_{\mathrm{on}}}{2}\sigma_z \nabla\cdot\mathbf{u}(\mathbf{r}),$$

$$\mathcal{H}^{\mathrm{K}'} = v_{\mathrm{F}}\boldsymbol{\sigma}'\cdot(\hat{\mathbf{p}} - \mathbf{A}^{\mathrm{q}}(\mathbf{r})) + \frac{g_{\mathrm{on}}}{2}\sigma_z \nabla\cdot\mathbf{u}(\mathbf{r}),$$

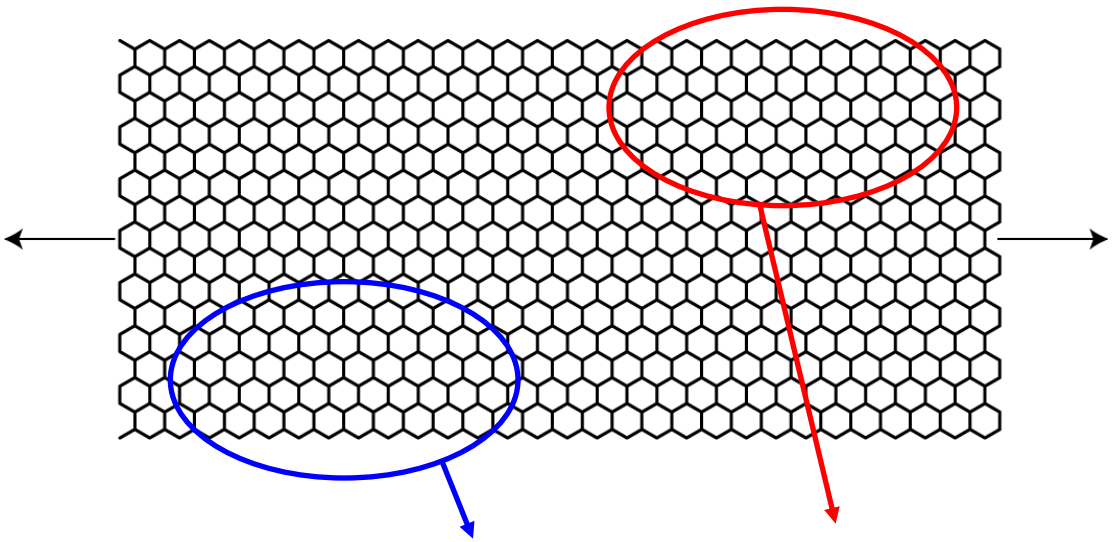
$$v_{\mathrm{F}}(A_x^{\mathrm{q}}(\mathbf{r}), A_y^{\mathrm{q}}(\mathbf{r})) = \frac{g_{\mathrm{off}}}{a_{\mathrm{cc}}}(u_y(\mathbf{r}), -u_x(\mathbf{r})),$$

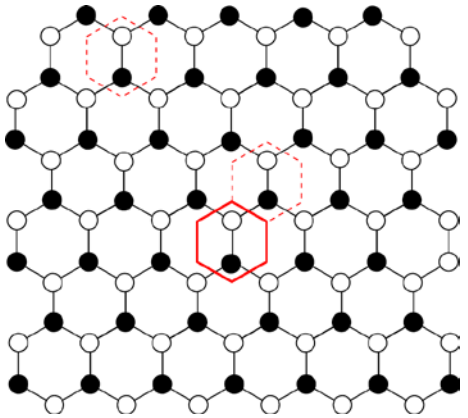
Ishikawa *et al*., JPSJ**75** (2006)

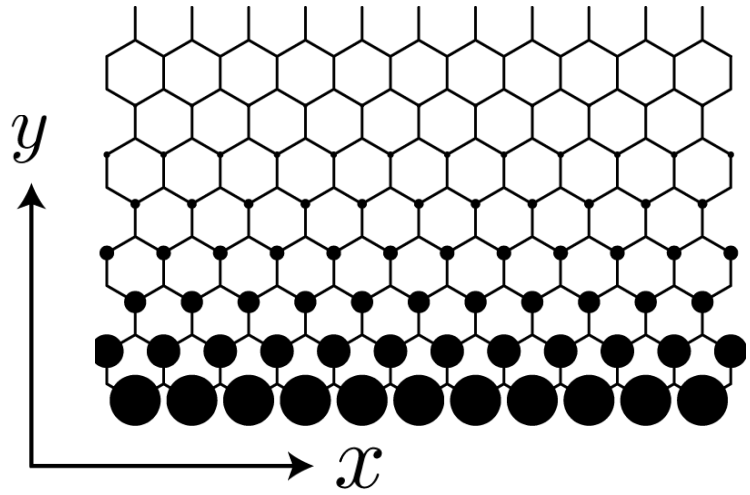
Sasaki *et al*., PRB**77** (2008)

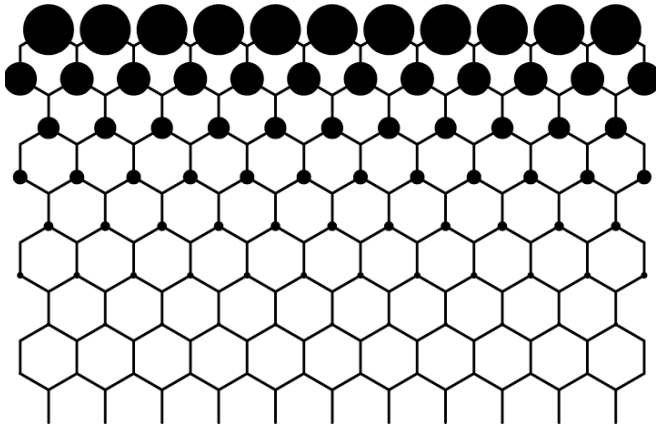


エッジ状態は擬スピンが傾いている

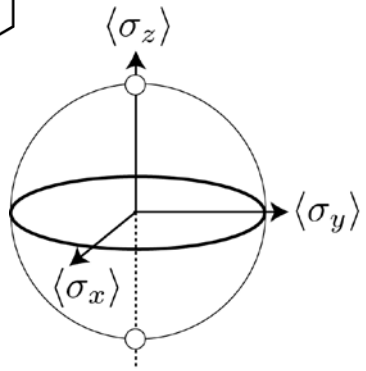


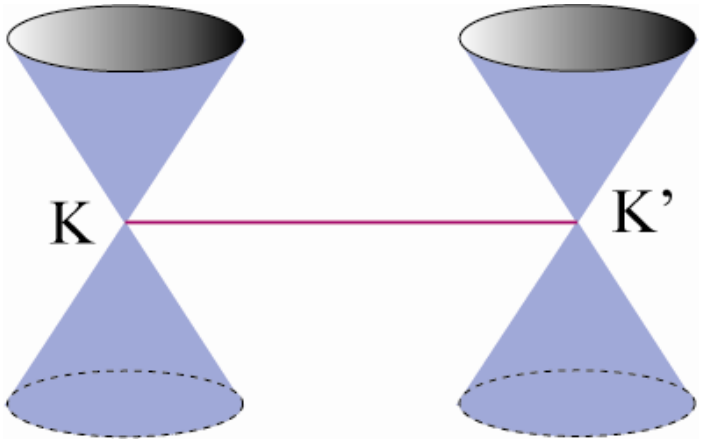






$$\begin{pmatrix} \Psi_{\mathrm{A}} \\ \Psi_{\mathrm{B}} \end{pmatrix} = N e^{-\frac{y}{\xi(k_x)}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

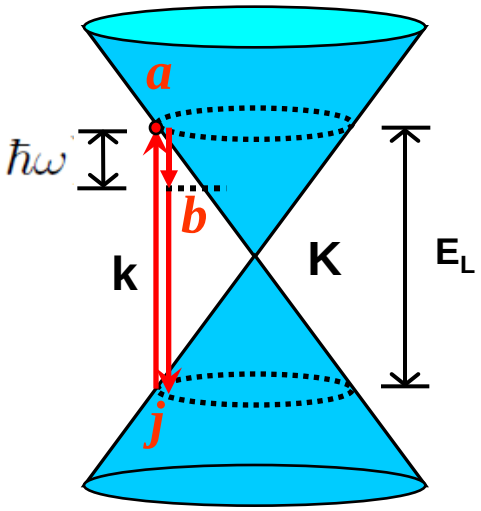




$$\begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = V$$

Calculation of G band Raman spectra

G band Raman spectra = Intensity + Spectral width



1. Raman Intensity $I(\omega, E_{\mathrm{L}})$

optical matrix · el-ph matrix · optical matrix · phonon energy

$$I(\omega, E_{\mathrm{L}}) = \sum_j \left| \sum_a \frac{M_{\mathrm{op}}(j,b) M_{\mathrm{el-ph}}(b,a) M_{\mathrm{op}}(a,j)}{\Delta E_{aj}(\Delta E_{aj} - \hbar\omega)} \right|^2$$

$$\Delta E_{aj} \equiv E_{\mathrm{L}} - (E_a - E_j) - i\gamma$$

Laser energy · resonance window

Phonon energy

$$\hbar\omega = \hbar\omega^{(0)} + \hbar\omega^{(2)}$$

Original frequency · Correction frequency Including el-ph coupling

2. Spectral width

Electron-hole pair creation matrix by el-ph interaction

$$\hbar\omega^{(2)} = 2\sum_{\mathbf{k}} \frac{|\langle eh(\mathbf{k})|H_{\mathrm{el-ph}}|\omega^{(0)}\rangle|^2}{\hbar\omega^{(0)} - [E_e(\mathbf{k}) - E_h(\mathbf{k})] + i\Gamma} \{f[E_e\mathbf{k}) - E_F] - f[E_h(\mathbf{k}) - E_F]\}$$

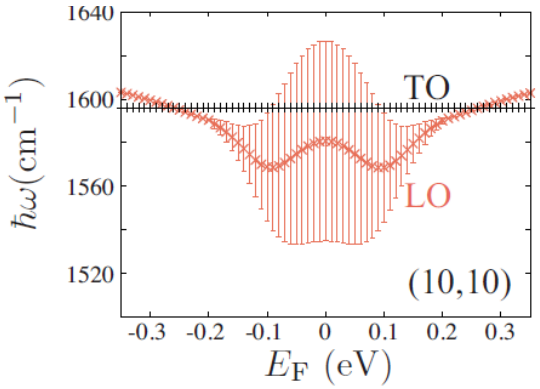
electron energy · hole energy · Spectral width · Fermi distribution function

K. Sasaki, *et al.* Phys. Rev. B 77, 245441 (2008)

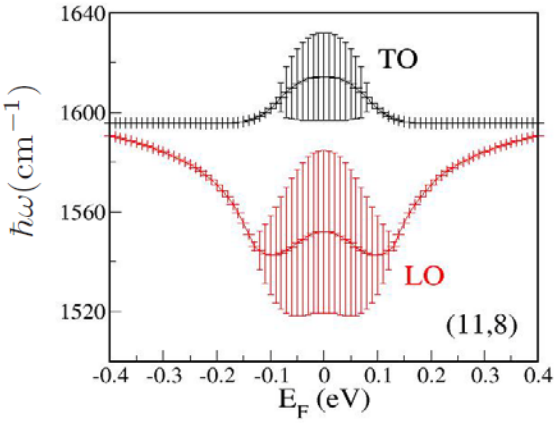
Spectral width is given by the decay length Γ.

Gate voltage dependence of G band Raman spectra

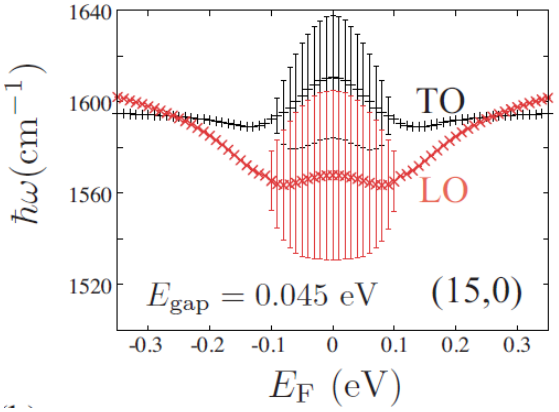
Armchair SWNT



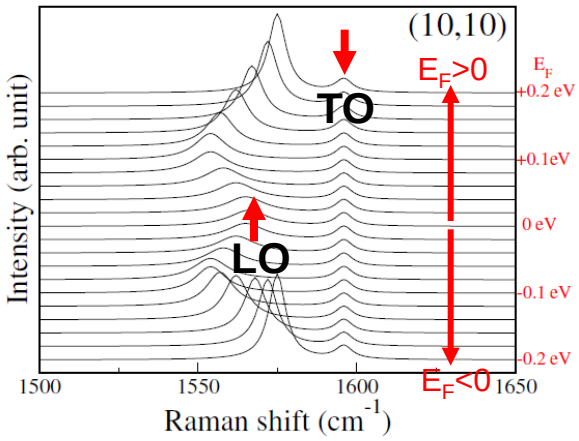
Chiral SWNT

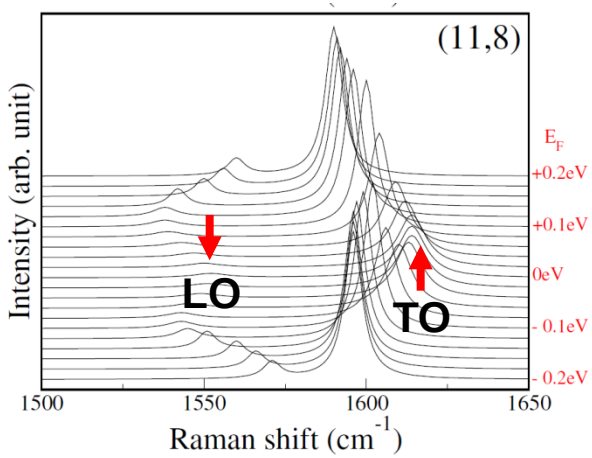


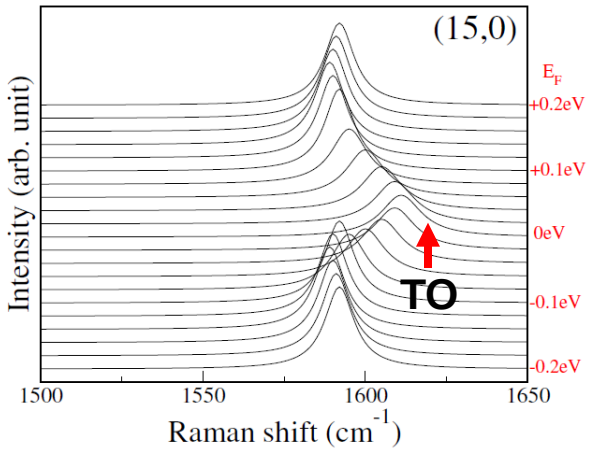
Zigzag SWNT



K. Sasaki, *et al.* Phys. Rev. B 77, 245441 (2008)



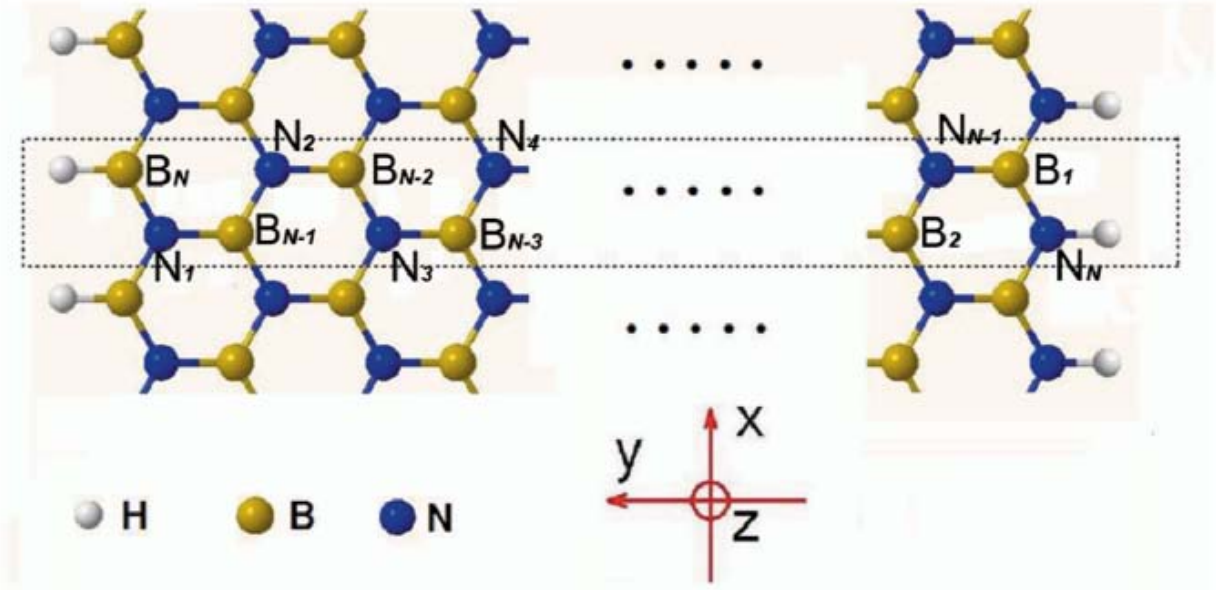




J. S. Park, *et al.* unpublished

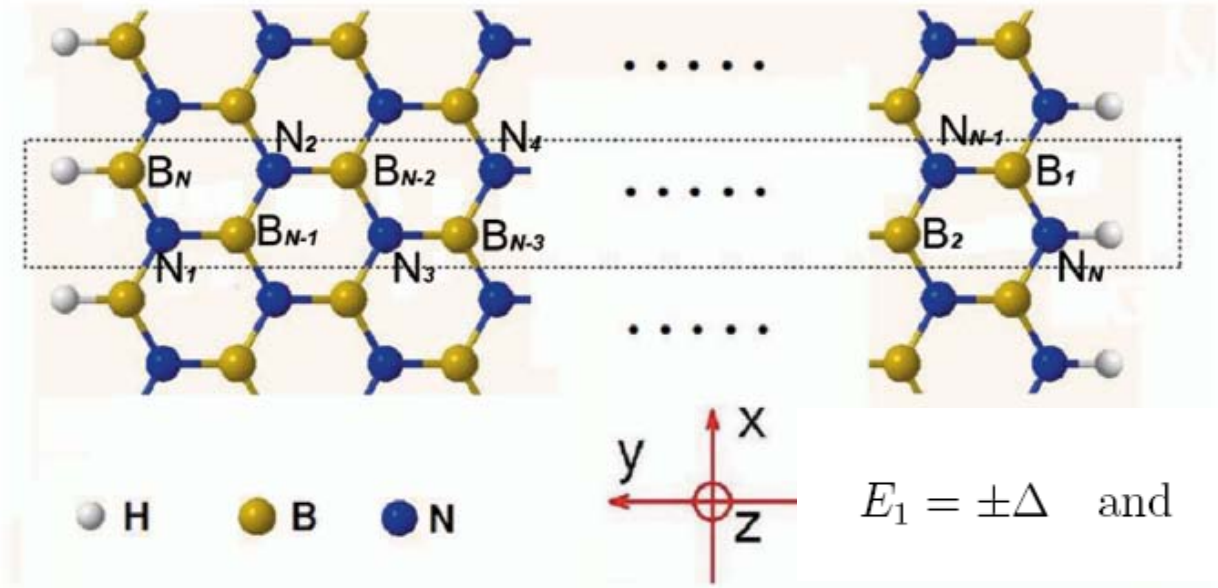
For LO mode of zigzag tube,
Electron-phonon coupling
→ Almost zero

BN nano ribbon



Zigzag BN nanoribbon

F. Zheng et al. (unpublished)



Zone boundary

$k = \pi/a$, $f = 0$

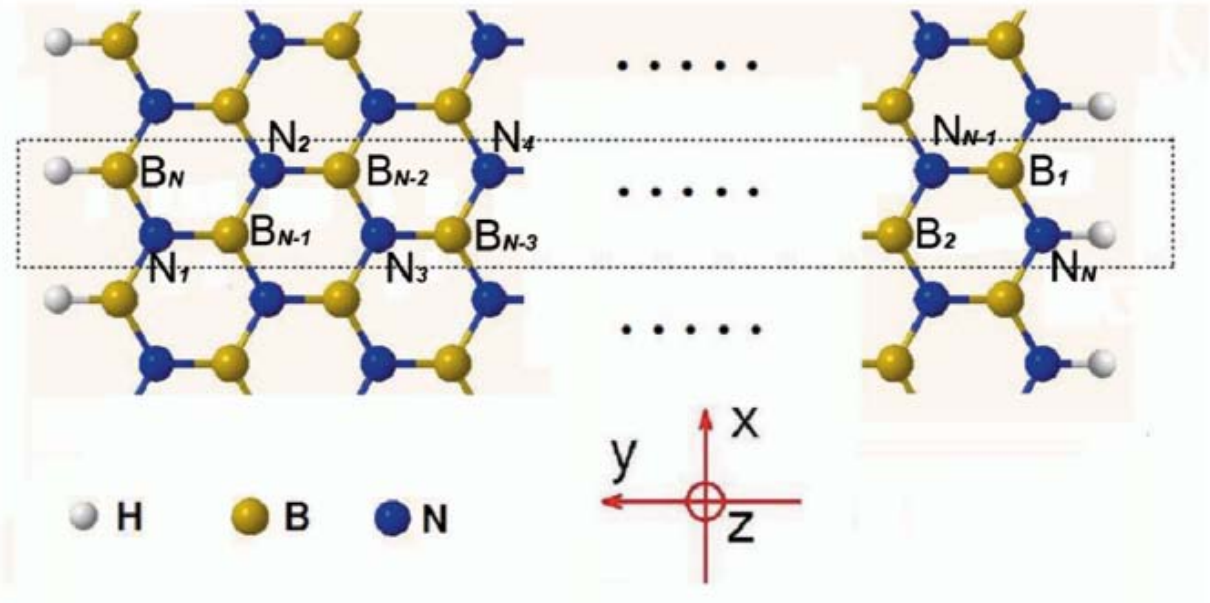
$$E_1 = \pm\Delta \quad \text{and} \quad E_2 = \frac{st \pm \sqrt{t^2 + \Delta^2 - s^2\Delta^2}}{s^2 - 1},$$

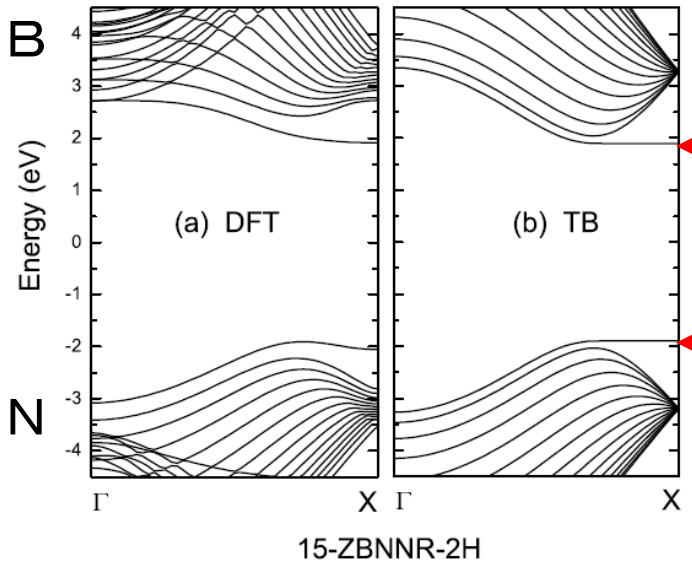
$$H = \begin{bmatrix} \Delta & tf & 0 & 0 & & \\ tf & -\Delta & t & 0 & \dots & \\ 0 & t & \Delta & tf & & \\ 0 & 0 & tf & -\Delta & \dots & \\ & \dots & & \dots & & \\ & & & & \Delta & tf \\ & & & & tf & -\Delta \end{bmatrix}, \quad S = \begin{bmatrix} 1 & sf & 0 & 0 & & \\ sf & 1 & s & 0 & \dots & \\ 0 & s & 1 & sf & & \\ 0 & 0 & sf & 1 & \dots & \\ & \dots & & \dots & & \\ & & & & 1 & sf \\ & & & & sf & 1 \end{bmatrix}$$

$$f = 2\cos\left(\frac{ka}{2}\right)$$

Energy band of BN nanoribbon

F. Zheng et al. (unpublished)





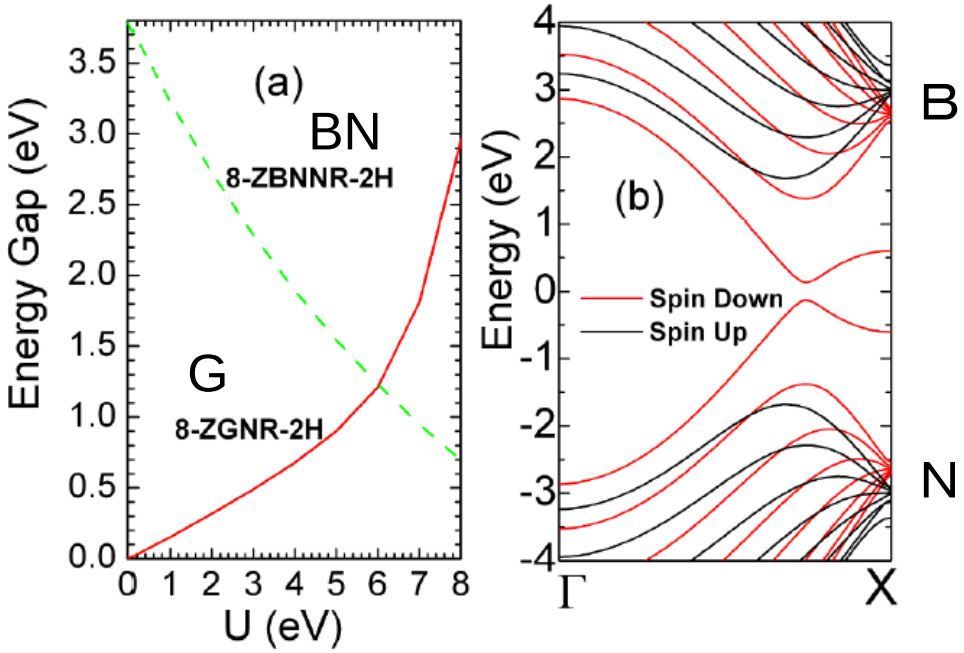
Edge state around B edge

Edge state around N edge

Pseudo spin polarized everywhere.

Coulomb interaction in BN ribbon

F. Zheng et al. (unpublished)



Energy gap decreases (BN)

increases (G)

One spin direction appears at E_F

$$U_B = U_N = 7.5\text{eV}$$

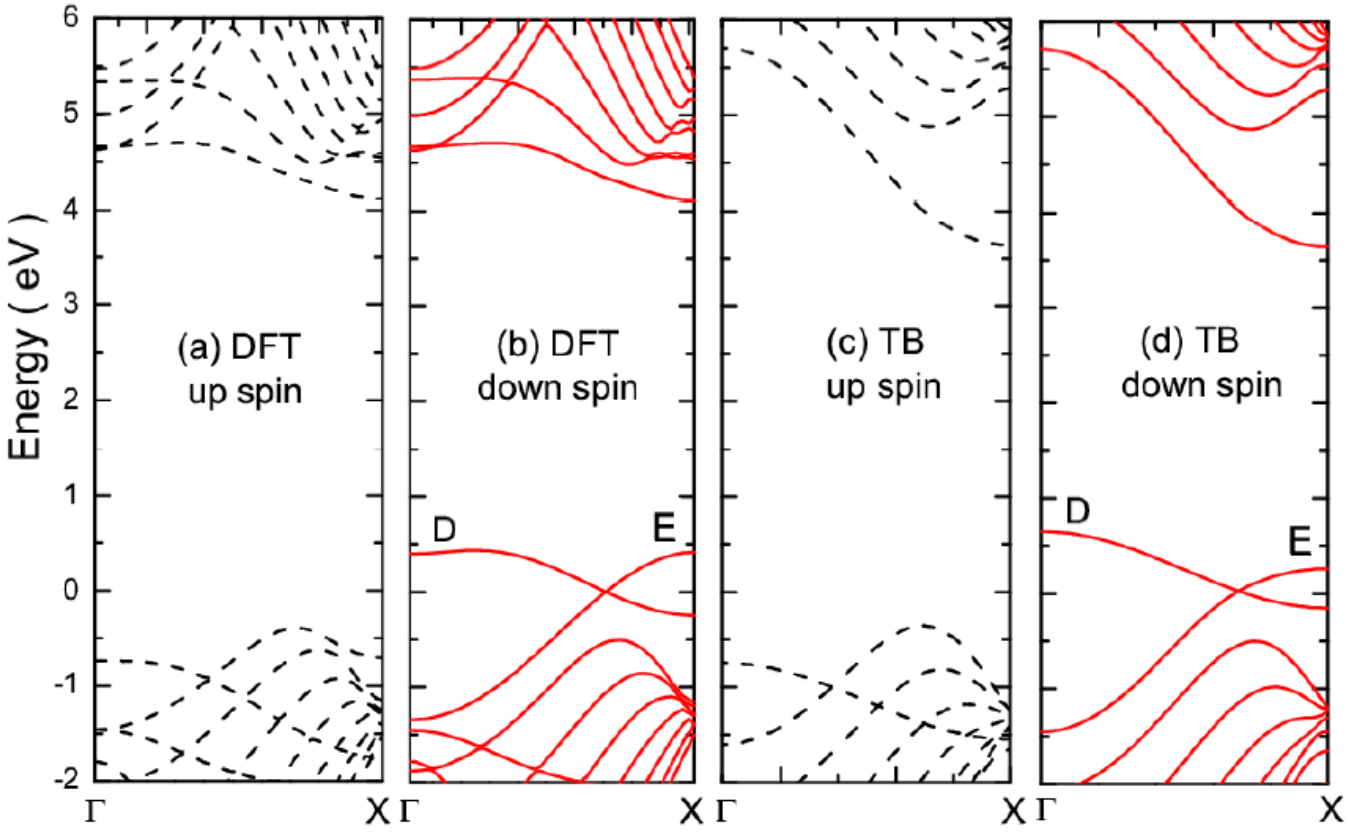
$$H = \sum_{i,\sigma} \Delta_i c^+_{i,\sigma} c_{i,\sigma} + \sum_{<i,j>,\sigma} t(c^+_{i,\sigma} c_{j,\sigma} + c^+_{j,\sigma} c_{i,\sigma}) + \sum_i U_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow},$$

$$\Delta_i = \begin{cases} \Delta & \text{boron} \\ -\Delta & \text{nitrogen} \end{cases}, \qquad U_i = \begin{cases} U_B & \text{boron} \\ U_N & \text{nitrogen} \end{cases}.$$

Half metalicity in BN ribbon

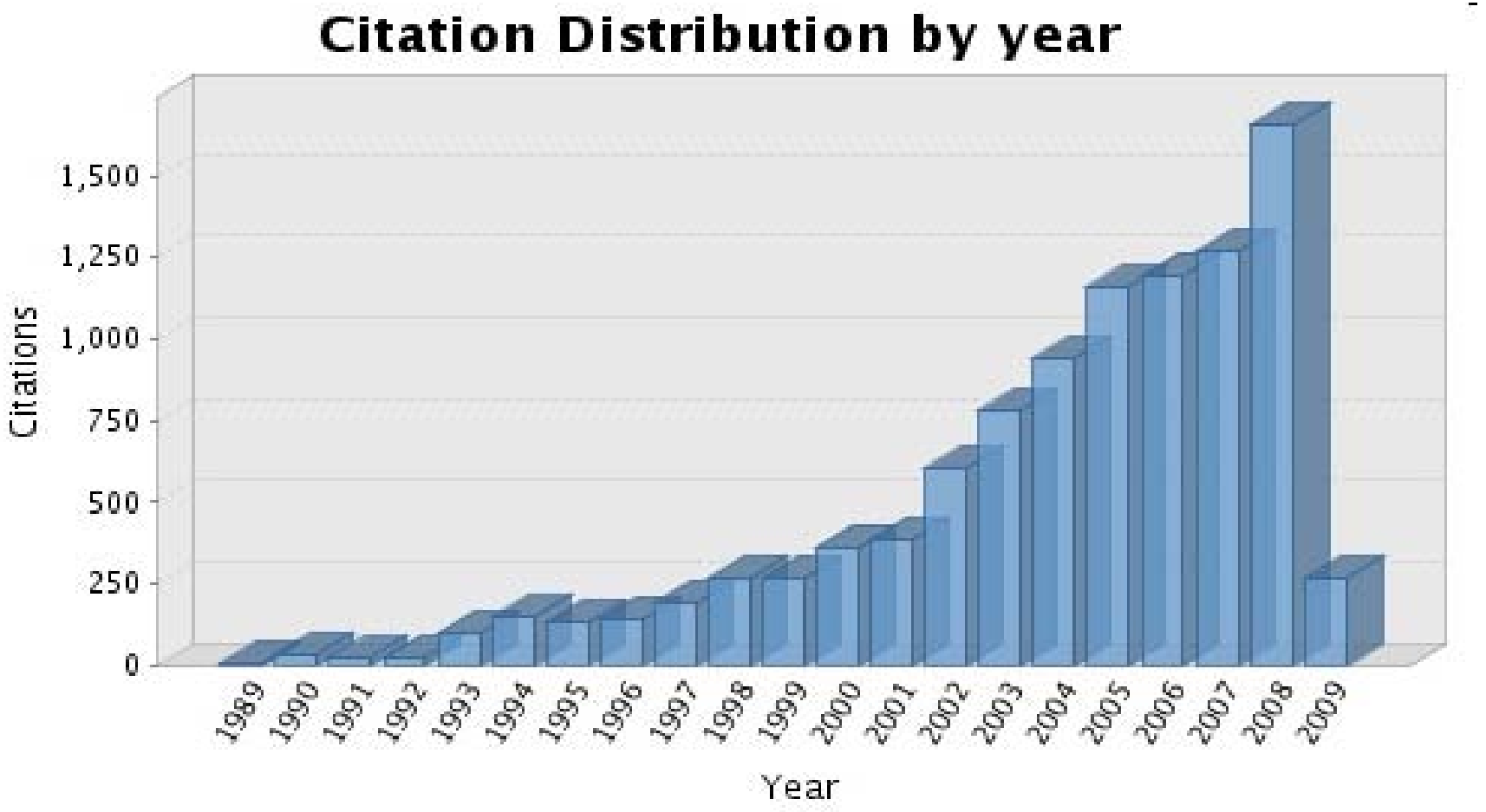
F. Zheng et al. (unpublished)

- Only down spin can flow at N zigzag edge
  - Half metalicity



D: dangling bond

E: edge states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