

ISSP International Summer School for Young Researchers on  
“Quantum Transport in Mesoscopic Scale & Low Dimensions”  
Aug. 13 - 21, 2003. (My talk is given at 16 Aug. 2003.)

## Electrical Conduction in Carbon Nanotubes

T. Nakanishi (AIST)

### 1. What is Carbon Nanotubes?

Quasi-one dimensional system

### 2. Effective-Mass Scheme

Electronic properties of carbon nanotubes

### 3. Impurity Scattering

Ballistic transport

(Absence of back-scattering for Slowly varying potential)

### 4. Point defects

### 5. Topological defect

### 6. Conclusion

#### Collaborators

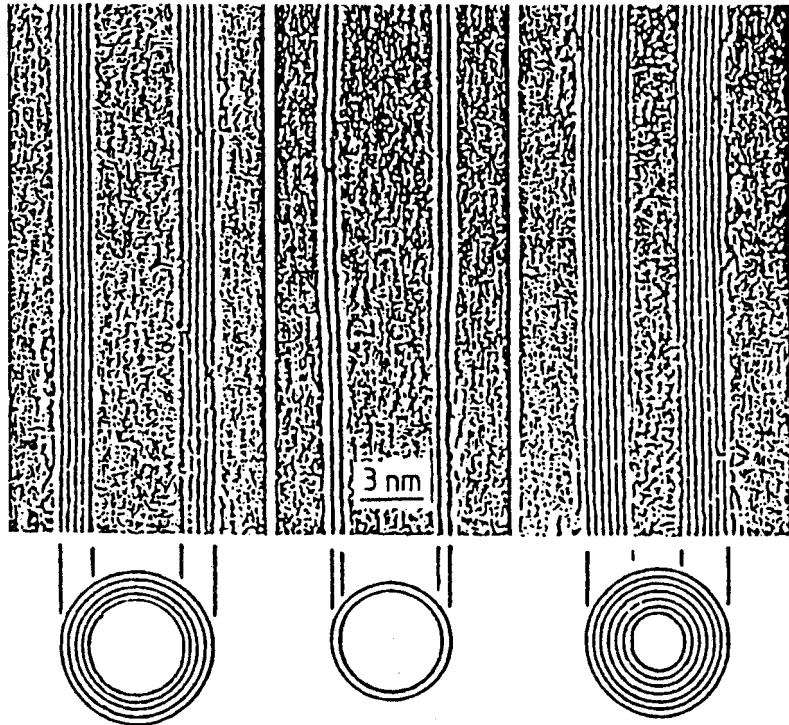
Tsuneya Ando (TIT)

Masatsura Igami (NISTEP)

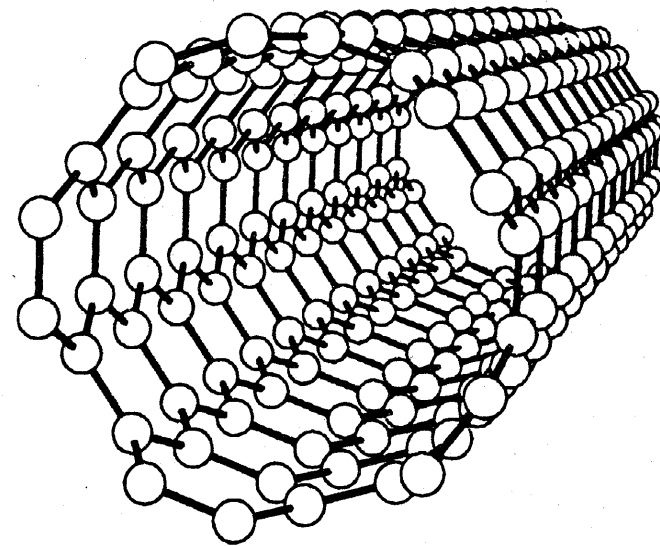
Riichiro Saito (Tohoku Univ.)

# Carbon Nanotubes

## Multi-wall



## Single-wall



Quantum wire growing naturally

Electron micrographs of CN

S. Iijima, Nature 354, 56 (1991)

Length  $\sim 1\mu m$

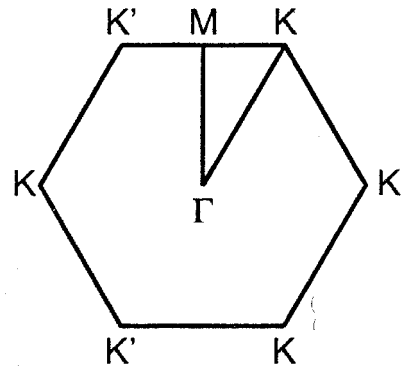
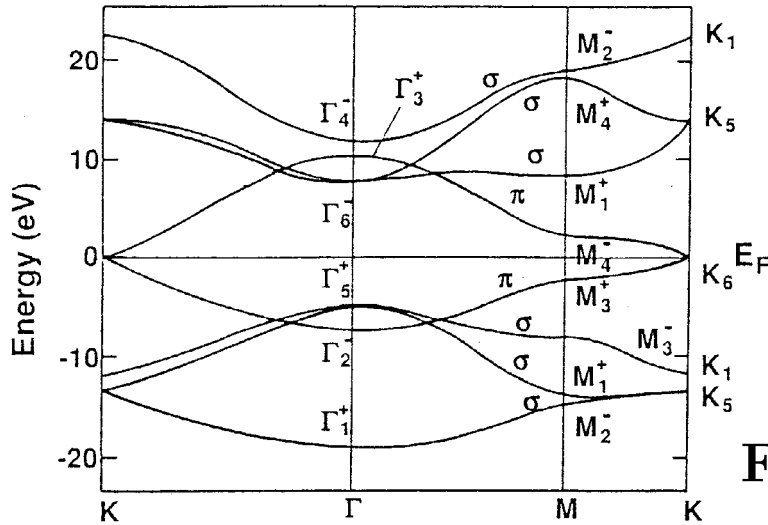
Diameter  $2 \sim 30nm$

Diameter  $\sim 4 nm$

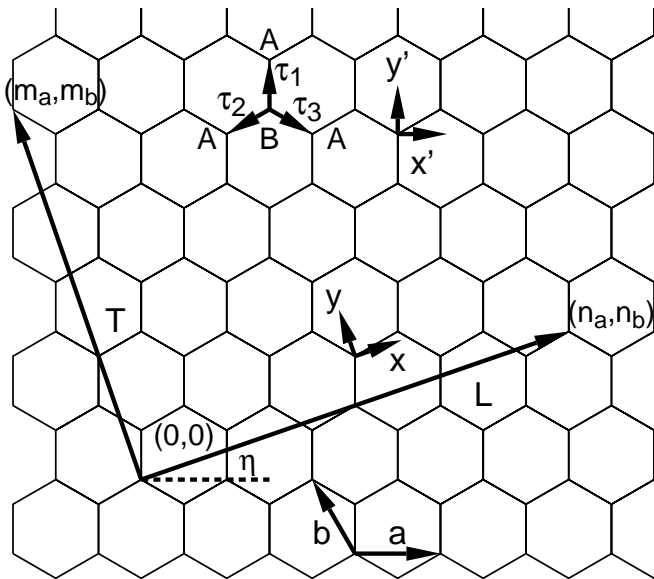
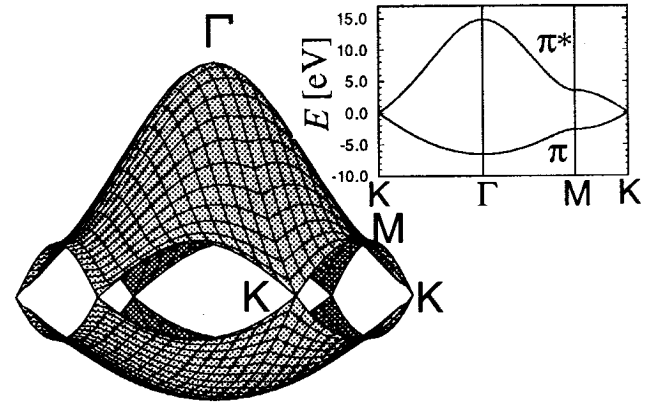
1D level spacing  $\sim 0.8 eV$

Graphene with periodic  
boundary condition

# Graphite sheet (Graphene)



First Brillouin Zone



$sp^2$  covalent bonding  
single  $\pi$  band

tight-binding model

Nearest-neighbor

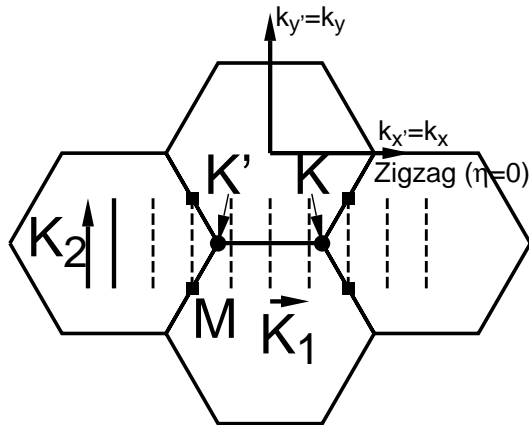
Transfer Integral:  $\gamma_0$

$$-\gamma_0 \sum_{l=1}^3 \psi_B(\mathbf{R}_A - \vec{\tau}_l) = \varepsilon \psi_A(\mathbf{R}_A),$$

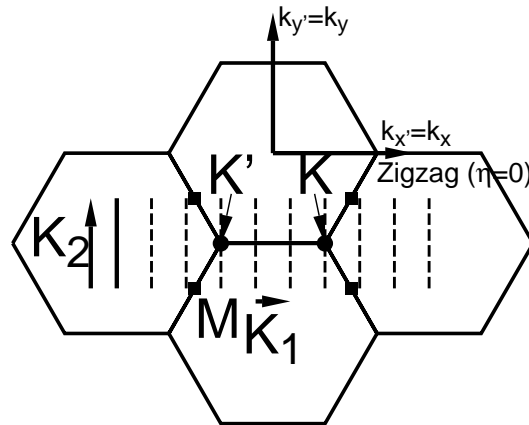
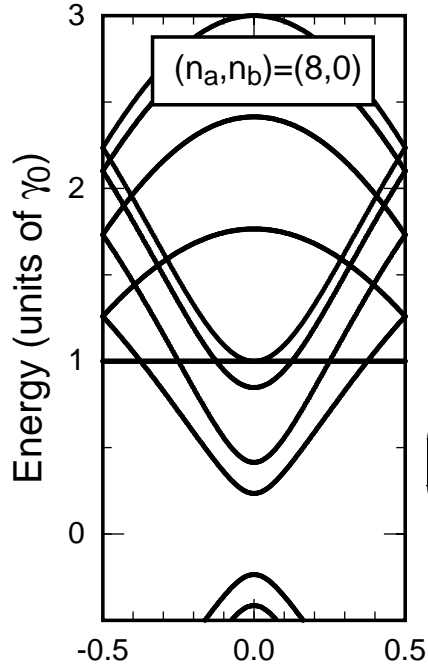
$$-\gamma_0 \sum_{l=1}^3 \psi_A(\mathbf{R}_B + \vec{\tau}_l) = \varepsilon \psi_B(\mathbf{R}_B).$$



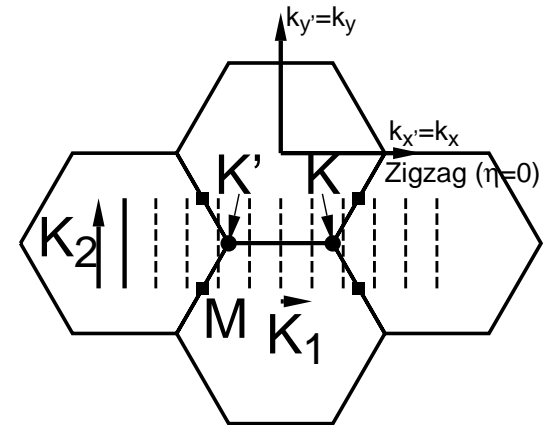
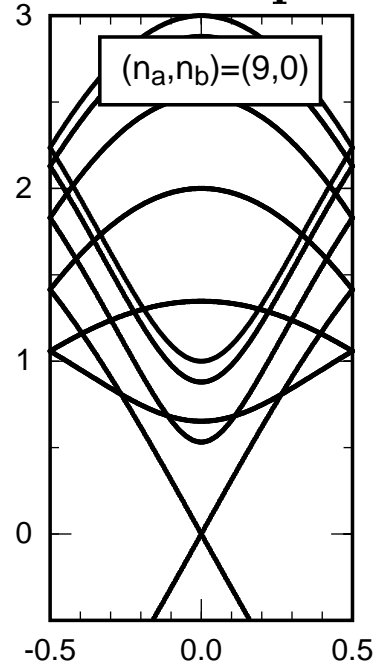
# Metallic and Semiconducting CN (Zigzag CN)



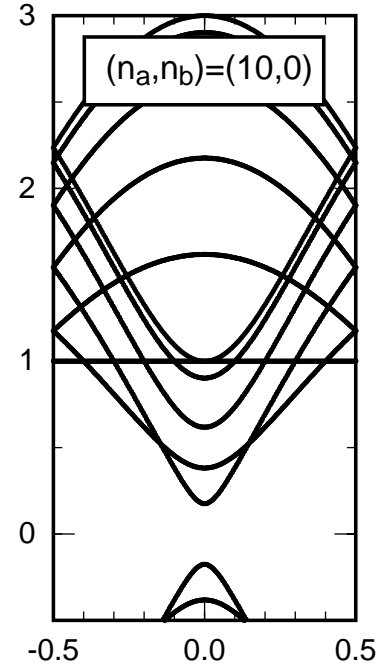
Semiconductor



Metal (Linear dispersion)



Semiconductor



$E_F = 0$

Wave Vector (units of  $2\pi/\sqrt{3}a$ )

## Effective-mass scheme

$$\mathbf{K} = (2\pi/a)(1/3, 1/\sqrt{3}), \quad \mathbf{K}' = (2\pi/a)(2/3, 0)$$

$$\begin{cases} \psi_A(\mathbf{R}_A) = \exp(i\mathbf{K} \cdot \mathbf{R}_A) F_A^K(\mathbf{R}_A) + e^{i\eta} \exp(i\mathbf{K}' \cdot \mathbf{R}_A) F_A^{K'}(\mathbf{R}_A), \\ \psi_B(\mathbf{R}_B) = -\omega e^{i\eta} \exp(i\mathbf{K} \cdot \mathbf{R}_B) F_B^K(\mathbf{R}_B) + \exp(i\mathbf{K}' \cdot \mathbf{R}_B) F_B^{K'}(\mathbf{R}_B), \end{cases}$$

$F_{A,B}^{K,K'}(\mathbf{R}_{A,B})$ : Envelope Functions

$$\omega = \exp(2\pi i/3)$$

— tight-binding model —

$$\begin{aligned} -\gamma_0 \sum_{l=1}^3 \psi_B(\mathbf{R}_A - \vec{\tau}_l) &= \varepsilon \psi_A(\mathbf{R}_A), \\ -\gamma_0 \sum_{l=1}^3 \psi_A(\mathbf{R}_B + \vec{\tau}_l) &= \varepsilon \psi_B(\mathbf{R}_B). \end{aligned}$$

$$F_B^{K,K'}(\mathbf{R}_A - \vec{\tau}_l) = F_B^{K,K'}(\mathbf{R}_A) - \vec{\tau}_l \cdot \frac{\partial}{\partial r_l} F_B^{K,K'}(\mathbf{R}_A)$$

$$F_A^{K,K'}(\mathbf{R}_B - \vec{\tau}_l) = F_A^{K,K'}(\mathbf{R}_B) - \vec{\tau}_l \cdot \frac{\partial}{\partial r_l} F_A^{K,K'}(\mathbf{R}_B)$$

**k·p approximation**

# Effective-Mass Equation

**k·p Hamiltonian**

**K point**

$$\begin{pmatrix} 0 & \gamma(\hat{k}_x - i\hat{k}_y) \\ \gamma(\hat{k}_x + i\hat{k}_y) & 0 \end{pmatrix} \begin{pmatrix} F_K^A \\ F_K^B \end{pmatrix} = \varepsilon \begin{pmatrix} F_K^A \\ F_K^B \end{pmatrix}$$

$$\gamma(\sigma_x \hat{k}_x + \sigma_y \hat{k}_y) \mathbf{F}_K(r) = \varepsilon \mathbf{F}_K(r)$$

**Weyl's equation for neutrinos**

**Band Parameter:**  $\gamma = \sqrt{3}a\gamma_0/2$

**Transfer Integral:**  $\gamma_0 \sim 2.6[\text{eV}]$

$$\hat{\mathbf{k}} = -i\vec{\nabla} + \frac{e}{c\hbar}\mathbf{A}$$

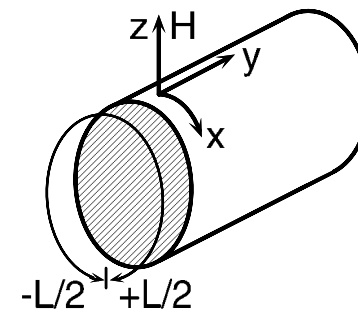
**Envelope Function:  $\mathbf{F}_K(r)$**

$$\mathbf{F}_K(r) = \begin{pmatrix} F_K^A \\ F_K^B \end{pmatrix}$$

**K' point**

$$\gamma(\sigma_x \hat{k}_x - \sigma_y \hat{k}_y) \mathbf{F}'_K(r) = \varepsilon \mathbf{F}'_K(r)$$

**Periodic Boundary Condition in  $x$  direction**



# Electronic States of CN's

## Wave functions

$$\mathbf{F}_K(r) = \frac{1}{\sqrt{2}} \begin{pmatrix} b_\nu(n, k_y) \\ \pm 1 \end{pmatrix} \exp [i\kappa_\nu(n)x + ik_y y]$$

$$\mathbf{F}_{K'}(r) = \frac{1}{\sqrt{2}} \begin{pmatrix} b_{-\nu}(n, k_y)^* \\ \pm 1 \end{pmatrix} \exp [i\kappa_{-\nu}(n)x + ik_y y]$$

with

$$n_a + n_b = 3N + \nu$$

$$b_\nu(n, k_y) = \frac{\kappa_\nu(n) - ik_y}{\sqrt{\kappa_\nu(n)^2 + k_y^2}}$$

## Energy levels

$$\varepsilon_\nu^\pm(n) = \pm\gamma\sqrt{\kappa_\nu(n)^2 + k_y^2}$$

**Discretized wave number in circumference direction**

$$k_x = \kappa_\nu(n) = \frac{2\pi}{L}(n - \nu/3)$$

Ajiki and Ando, J. Phys. Soc. Jpn., 62, 1255 (1993)

$\nu = 0$     **metallic CN**

**Linear dispersion**

$$\varepsilon_0^\pm(0) = \pm\gamma|k_y|$$

$\nu = \pm 1$     **semiconducting CN**

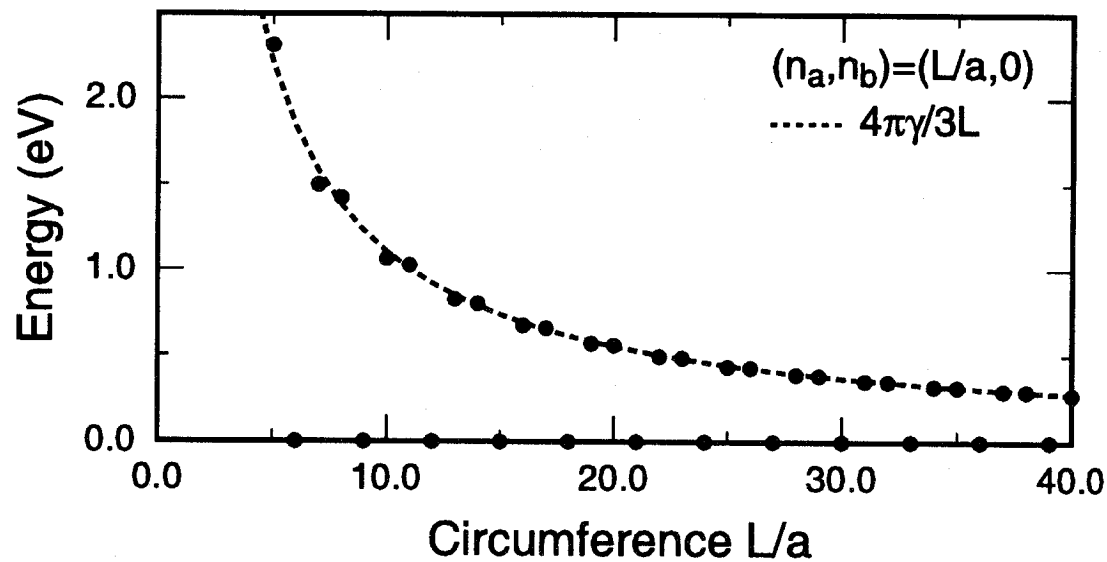
**Band gap**

$$E_g = 2\gamma|\kappa_{\pm 1}(0)| = \frac{4\pi\gamma}{3L}$$

## Band Gap

$$E_g = \frac{4\pi\gamma}{3L}$$

### Band Gap of Zigzag Nanotubes



M. S. Dresselhaus, G. Dresselhaus and R. Saito, Sol. State Com., **84**, 201 (1992).

H. Ajiki and T. Ando, J. Phys. Soc. Jpn., **62**, 1255 (1993).

## Effective–Potential

T. Ando and T. Nakanishi, J. Phys. Soc. Jpn. **67**,1704 (1998)

Effective–Mass Equation

$$(\mathcal{H}_0 + V)\mathcal{F} = \varepsilon\mathcal{F}$$

$$\mathcal{H}_0 = \begin{pmatrix} 0 & \gamma(\hat{k}_x - i\hat{k}_y) & 0 & 0 \\ \gamma(\hat{k}_x + i\hat{k}_y) & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma(\hat{k}_x + i\hat{k}_y) \\ 0 & 0 & \gamma(\hat{k}_x - i\hat{k}_y) & 0 \end{pmatrix}, \mathcal{F} = \begin{pmatrix} F_A^K(\mathbf{r}) \\ F_B^K(\mathbf{r}) \\ F_A^{K'}(\mathbf{r}) \\ F_B^{K'}(\mathbf{r}) \end{pmatrix}$$

$$V = \begin{pmatrix} u_A(\mathbf{r}) & 0 & e^{i\eta}u'_A(\mathbf{r}) & 0 \\ 0 & u_B(\mathbf{r}) & 0 & -\omega^{-1}e^{-i\eta}u'_B(\mathbf{r}) \\ e^{-i\eta}u'_A(\mathbf{r})^* & 0 & u_A(\mathbf{r}) & 0 \\ 0 & -\omega e^{i\eta}u'_B(\mathbf{r})^* & 0 & u_B(\mathbf{r}) \end{pmatrix}$$

$$u_A = \frac{\sqrt{3}a^2}{2} \sum_{\mathbf{R}_A} \tilde{u}_A(\mathbf{R}_A),$$

$$u_B = \frac{\sqrt{3}a^2}{2} \sum_{\mathbf{R}_B} \tilde{u}_B(\mathbf{R}_B),$$

$$u'_A = \frac{\sqrt{3}a^2}{2} \sum_{\mathbf{R}_A} e^{i(\mathbf{K}' - \mathbf{K}) \cdot \mathbf{R}_A} \tilde{u}_A(\mathbf{R}_A),$$

$$u'_B = \frac{\sqrt{3}a^2}{2} \sum_{\mathbf{R}_B} e^{i(\mathbf{K}' - \mathbf{K}) \cdot \mathbf{R}_B} \tilde{u}_B(\mathbf{R}_B),$$

$\sqrt{3}a^2/2$ : Area of a Unit Cell

Slowly-varying Potential

Potential Range  $d \gg a$

$$u_A(\mathbf{r}) = u_B(\mathbf{r})$$

$$u'_A(\mathbf{r}) = u'_B(\mathbf{r}) = 0$$

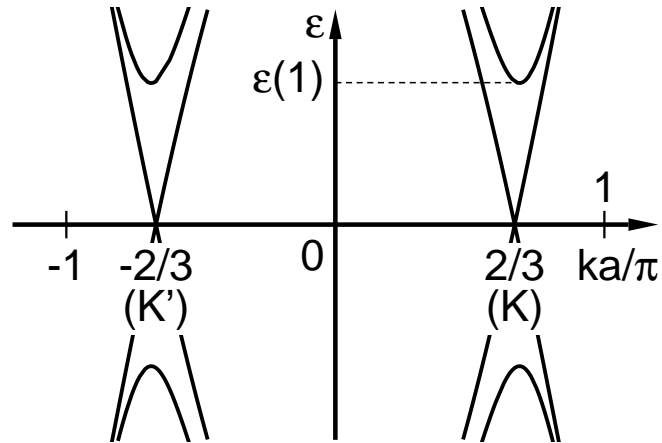
Potential Range  $d \ll$  Circumference  $L = |\mathbf{L}|$

$$u_A(\mathbf{r}) = u_A \delta(\mathbf{r} - \mathbf{r}_0), \quad u_B(\mathbf{r}) = u_B \delta(\mathbf{r} - \mathbf{r}_0),$$

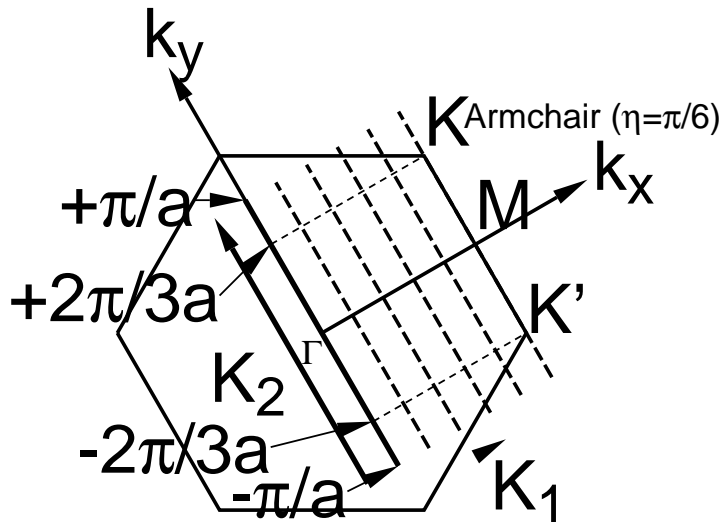
$$u'_A(\mathbf{r}) = u'_A \delta(\mathbf{r} - \mathbf{r}_0), \quad u'_B(\mathbf{r}) = u'_B \delta(\mathbf{r} - \mathbf{r}_0).$$

$\mathbf{r}_0$  : Impurity Position

## Right- and left-going channels



Metallic CN



$(n_a, n_b) = (2, 1)m$   
armchair CN

○ Solutions for  $V = 0, |\epsilon| < \epsilon(1) = \frac{2\pi\gamma}{L}$

$$\mathbf{F}^{K\pm} = \begin{pmatrix} F_A^K(\mathbf{r}) \\ F_B^K(\mathbf{r}) \end{pmatrix} = \frac{1}{\sqrt{2AL}} \begin{pmatrix} \mp i \\ 1 \end{pmatrix} \exp(iky),$$

$$\mathbf{F}^{K'\pm} = \begin{pmatrix} F_A^{K'}(\mathbf{r}) \\ F_B^{K'}(\mathbf{r}) \end{pmatrix} = \frac{1}{\sqrt{2AL}} \begin{pmatrix} \pm i \\ 1 \end{pmatrix} \exp(iky).$$

$A$ : Length of Nanotube

Energy:  $\epsilon(k) = \pm\gamma k$

Group Velocity:  $v = \pm\gamma/\hbar$

$$\pm \begin{cases} \text{Right-going } \mathbf{F}^{K+}, \mathbf{F}^{K'+} \\ \text{Left-going } \mathbf{F}^{K-}, \mathbf{F}^{K'-} \end{cases}$$

## Lowest Born Approximation

### ○ Inter-valley Scattering

$$\begin{aligned}
 V_{K\pm K'+} &= \frac{1}{2AL} \int d\mathbf{r} \begin{pmatrix} \pm i & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} e^{i\eta} u'_A(\mathbf{r}) & 0 \\ 0 & -\omega^{-1} e^{-i\eta} u'_B(\mathbf{r}) \end{pmatrix} \begin{pmatrix} i \\ 1 \end{pmatrix} \\
 &= \frac{1}{2AL} \int d\mathbf{r} \{ \mp e^{i\eta} u'_A(\mathbf{r}) - \omega^{-1} e^{-i\eta} u'_B(\mathbf{r}) \} \\
 &= \frac{1}{2AL} (\mp u'_A e^{i\eta} - \omega^{-1} e^{-i\eta} u'_B) = V_{K'\pm K+}^*
 \end{aligned}$$

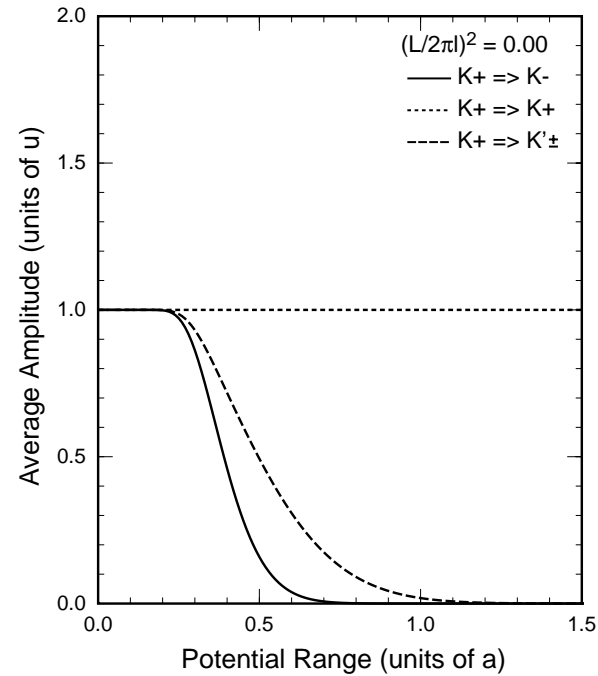
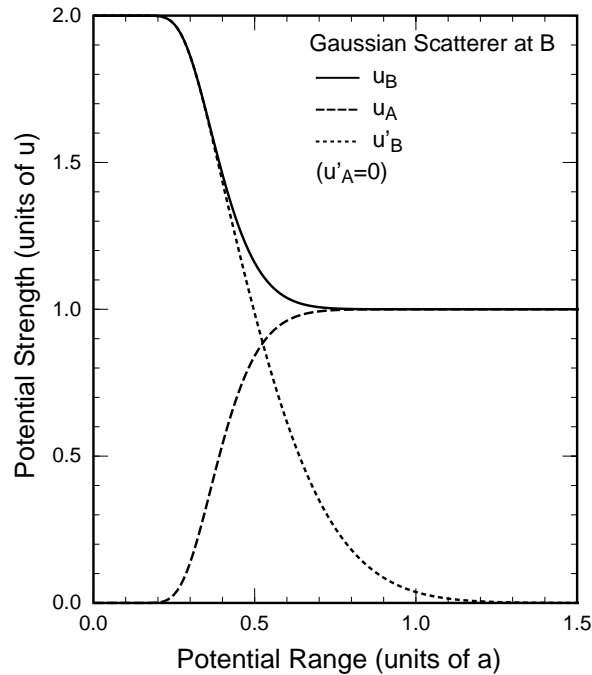
### ○ Intra-valley Scattering

$$\begin{aligned}
 V_{K\pm K+} &= \frac{1}{2AL} \int d\mathbf{r} \begin{pmatrix} \pm i & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} u_A(\mathbf{r}) & 0 \\ 0 & u_B(\mathbf{r}) \end{pmatrix} \begin{pmatrix} -i \\ 1 \end{pmatrix} \\
 &= \frac{1}{2AL} \int d\mathbf{r} \{ \pm u_A(\mathbf{r}) + u_B(\mathbf{r}) \} \\
 &= \frac{1}{2AL} (\pm u_A + u_B) = V_{K'\pm K'+}
 \end{aligned}$$

**Absence of back-scattering for slowly varying potential**

$$V_{K-K'+} = V_{K'-K+}^* = 0, \quad V_{K-K+} = V_{K'-K'+} \propto u_B - u_A = 0$$

# Gaussian Potential



$$V(\mathbf{r}) = \frac{f(d/a)u}{\pi d^2} \exp\left(-\frac{\mathbf{r}^2}{d^2}\right)$$

$f(d/a)$ : Normalization Factor

$$\sum_{i=A,B} \sum_{\mathbf{R}_i} \frac{\sqrt{3}a^2}{4} V(\mathbf{R}_i - \mathbf{R}_B^0) = u = (u_A + u_B)/2$$

$d \gg a$ : Absence of Back Scattering



Huge Conductivity,  
Quantized Conductance

# Magnetic Field

**Solutions for  $V = 0, |\varepsilon| < \varepsilon(1)$**

**Gauge:  $\mathbf{A} = (0, \frac{LH}{2\pi} \sin \frac{2\pi x}{L})$**

$$\mathbf{F}_{sk}^K = \begin{pmatrix} F_A^K(\mathbf{r}) \\ F_B^K(\mathbf{r}) \end{pmatrix} = \frac{1}{\sqrt{2A}} \begin{pmatrix} -is(k/|k|)F_-(x) \\ F_+(x) \end{pmatrix} \exp(iky),$$

$$\mathbf{F}_{sk}^{K'} = \begin{pmatrix} F_A^{K'}(\mathbf{r}) \\ F_B^{K'}(\mathbf{r}) \end{pmatrix} = \frac{1}{\sqrt{2A}} \begin{pmatrix} +is(k/|k|)F_+(x) \\ F_-(x) \end{pmatrix} \exp(iky).$$

$$F_{\pm}(x) = \frac{1}{\sqrt{LI_0(\alpha)}} \exp \left[ \pm \frac{1}{2} \alpha \cos \frac{2\pi x}{L} \right]$$

$\alpha = 2 \left( \frac{L}{2\pi l} \right)^2$ : **Magnetic Field**

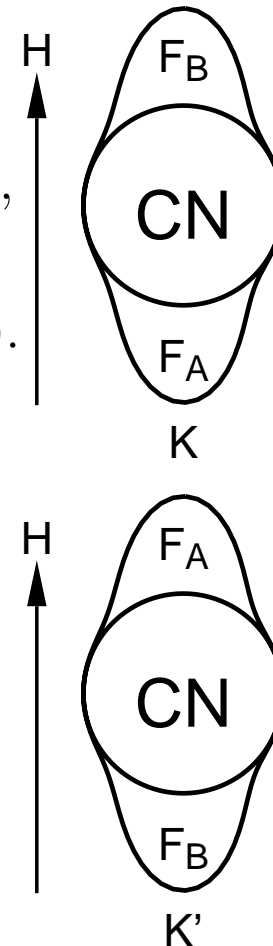
$l = \sqrt{c\hbar/eH}$ : **Magnetic Length**

$I_0(z)$ : **Modified Bessel function of the first kind**

$$I_0(z) = \int_0^\pi \frac{d\theta}{\pi} \exp(z \cos \theta)$$

$s = +1$  **conduction band**

$s = -1$  **valence band**



T. Ando and T. Seri, J. Phys. Soc.

Jpn. **66**,3558 (1997)

## Back scatterings in magnetic field

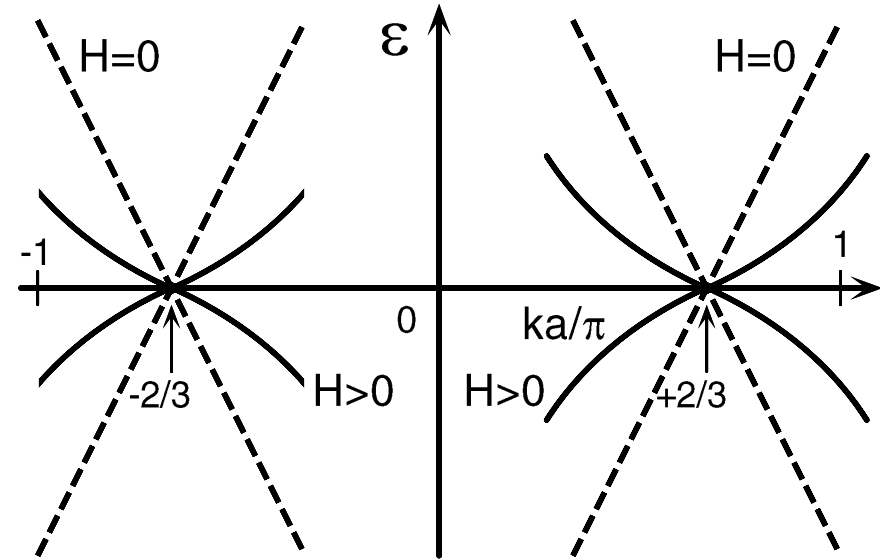
### Energy

$$\varepsilon(k) = s\gamma|k|I_0(\alpha)^{-1}$$

$(n_a, n_b) = (2, 1)m$  : armchair CN

Dashed lines:  $H = 0$

Solid lines:  $H \neq 0$



### Lowest Born Approximation

○ Inter-valley Scattering

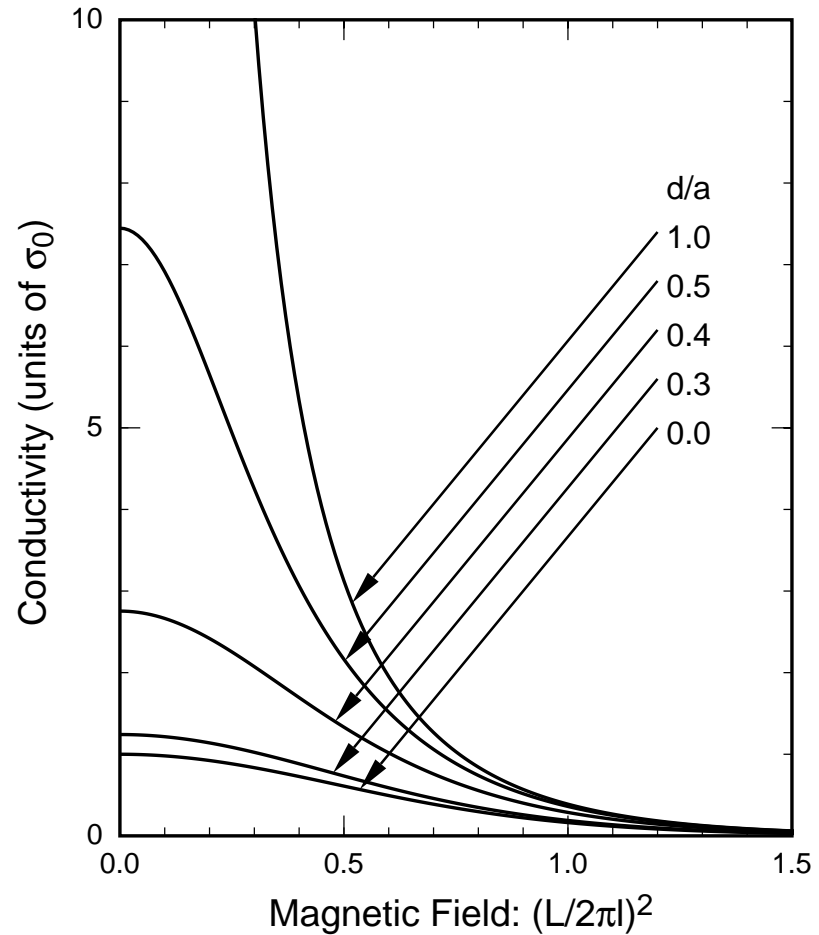
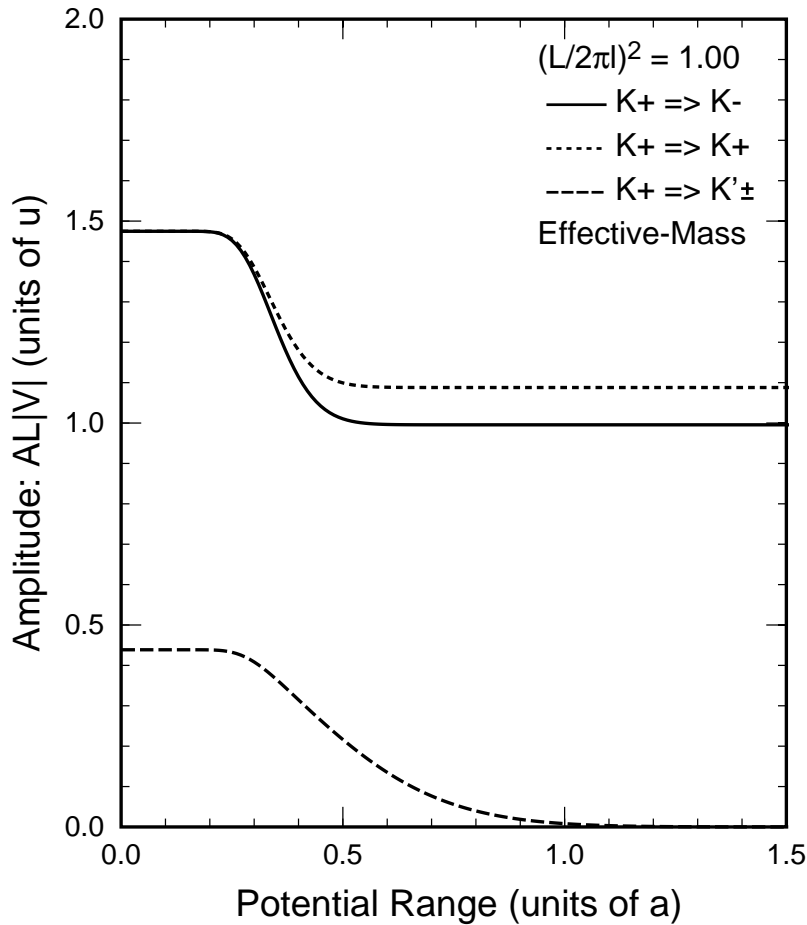
$$V_{K\pm K'_+} = \frac{1}{2A} (\mp u'_A e^{i\eta} - \omega^{-1} e^{-i\eta} u'_B) F_+(x_0) F_-(x_0) = V_{K'_\pm K_+}^*$$

○ Intra-valley Scattering

$$V_{K\pm K_+} = \frac{1}{2A} (\pm u_A F_-(x_0)^2 + u_B F_+(x_0)^2) = V_{K'_\pm K'_+}$$

# Dependence on the Magnetic Field

## Huge Positive Magnetoresistance



**Boltzmann conductivity**

$$\sigma_0 = \frac{e^2}{2\pi\hbar}\Lambda, \quad \Lambda = \frac{\tau\gamma}{\hbar}, \quad \frac{\hbar}{\tau} = \frac{4n_i\langle u^2 \rangle}{\gamma L}$$

## Absence of Back Scattering( $d \gg a$ )

$$T = V + V \frac{1}{\varepsilon - \mathcal{H}_0} V + V \frac{1}{\varepsilon - \mathcal{H}_0} V \frac{1}{\varepsilon - \mathcal{H}_0} V + \dots$$

$$\mathcal{H}_0 = \gamma \begin{pmatrix} 0 & \hat{k}_x - i\hat{k}_y \\ \hat{k}_x + i\hat{k}_y & 0 \end{pmatrix}$$

Long range Potential

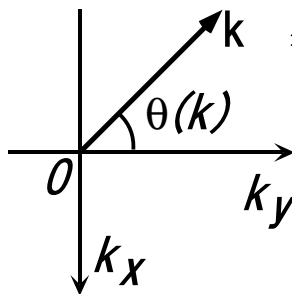
$$V = \begin{pmatrix} V(\mathbf{r}) & 0 \\ 0 & V(\mathbf{r}) \end{pmatrix}$$

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

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

$s = +1$  conduction band

$s = -1$  valence band



$$\varepsilon_s(-\mathbf{k}) = \varepsilon_s(\mathbf{k})$$

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

$$k_x + ik_y = i|\mathbf{k}|e^{i\theta(\mathbf{k})}$$

Spin-rotation operator

$$R(\theta) = \exp\left(i\frac{\theta}{2}\sigma_z\right)$$

$$= \begin{pmatrix} \exp(+i\theta/2) & 0 \\ 0 & \exp(-i\theta/2) \end{pmatrix}$$

$$|s\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -is \\ 1 \end{pmatrix}$$

# Absence of Back Scattering( $d \gg a$ )

T. Ando and T. Nakanishi, J. Phys. Soc. Jpn. **67**,1704 (1998)

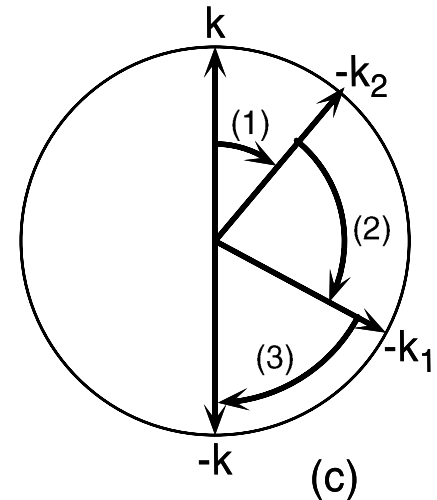
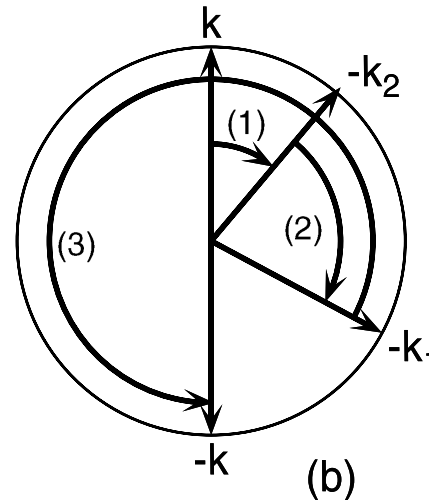
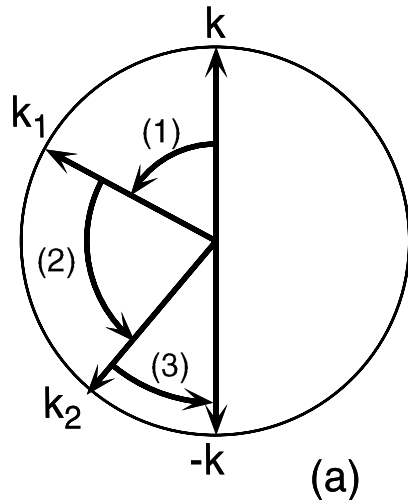
$(p+1)$ th order term

$$\begin{aligned}
 (s, -\mathbf{k} | T^{(p+1)} | s, +\mathbf{k}) &= \frac{1}{LA_{s_1 \mathbf{k}_1}} \frac{1}{LA_{s_2 \mathbf{k}_2}} \cdots \frac{1}{LA_{s_p \mathbf{k}_p}} \\
 &\times \frac{V(-\mathbf{k} - \mathbf{k}_p) \cdots V(\mathbf{k}_2 - \mathbf{k}_1) V(\mathbf{k}_1 - \mathbf{k})}{[\varepsilon - \varepsilon_{s_p}(\mathbf{k}_p)] \cdots [\varepsilon - \varepsilon_{s_2}(\mathbf{k}_2)] [\varepsilon - \varepsilon_{s_1}(\mathbf{k}_1)]} \\
 &\times e^{-i\phi_s(-\mathbf{k})} (s | R[\theta(-\mathbf{k})] R^{-1}[\theta(\mathbf{k}_p)] | s_p) \\
 &\times \cdots \times (s_2 | R[\theta(\mathbf{k}_2)] R^{-1}[\theta(\mathbf{k}_1)] | s_1) \\
 &\times (s_1 | R[\theta(\mathbf{k}_1)] R^{-1}[\theta(\mathbf{k})] | s) e^{i\phi_s(\mathbf{k})}
 \end{aligned}$$

**time-reversal terms  
cancel out**

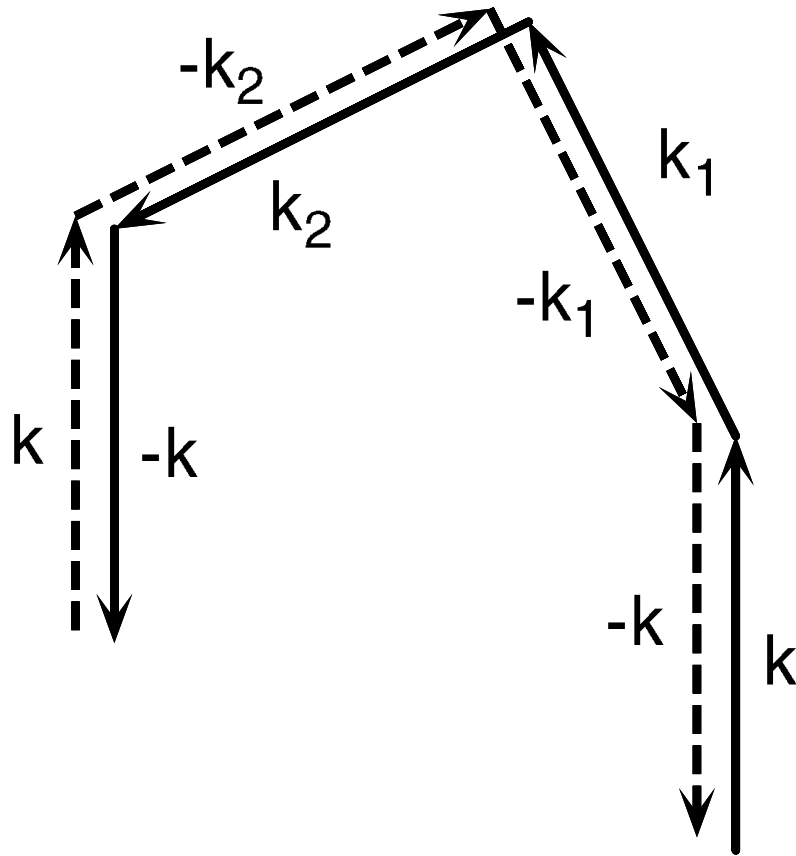
$$\begin{aligned}
 (s_1, k_1) &\rightarrow (s_p, -k_p), \\
 (s_2, k_2) &\rightarrow (s_{p-1}, -k_{p-1}), \cdots \\
 R[\theta] &= -R[\theta + 2\pi]
 \end{aligned}$$

$$\varepsilon_s(-\mathbf{k}) = \varepsilon_s(\mathbf{k})$$



# Berry's Phase and Absence of Back Scattering

T. Ando, T. Nakanishi, and R. Saito, J. Phys. Soc. Jpn. **67**,2857 (1998)



$$\psi_s(\mathbf{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} -is \\ \exp[i\theta(\mathbf{k})] \end{pmatrix}$$

$$\psi_s(\mathbf{k}) \longrightarrow \psi_s(\mathbf{k}) \exp(-i\varphi)$$

Berry's Phase

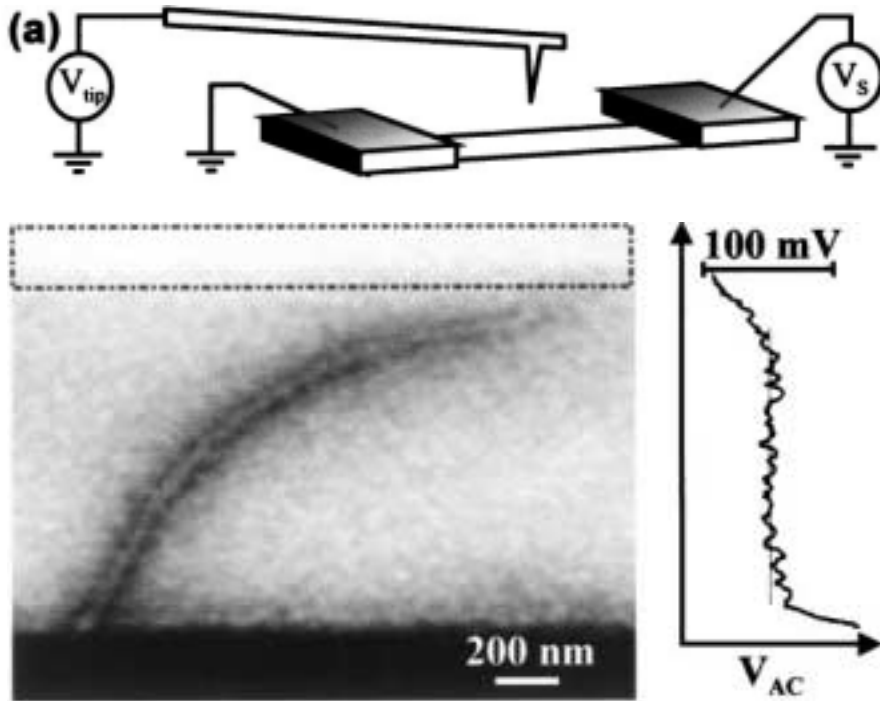
$$\varphi = -i \int_0^T dt \left\langle \psi_s[\mathbf{k}(t)] \left| \frac{d}{dt} \psi_s[\mathbf{k}(t)] \right. \right\rangle = \pi$$

$$R[\theta - 2\pi] = -R[\theta]$$

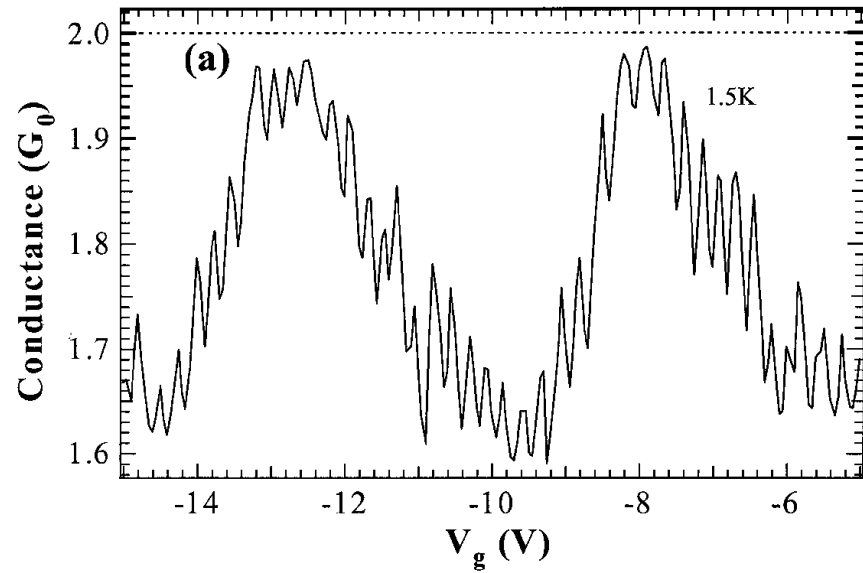
$$R[-\pi] = -R[\pi]$$

# Experiments

## 0 Voltage Drop



Good Contact  $2G_0 = 4e^2/h$   
Almost perfect transmission



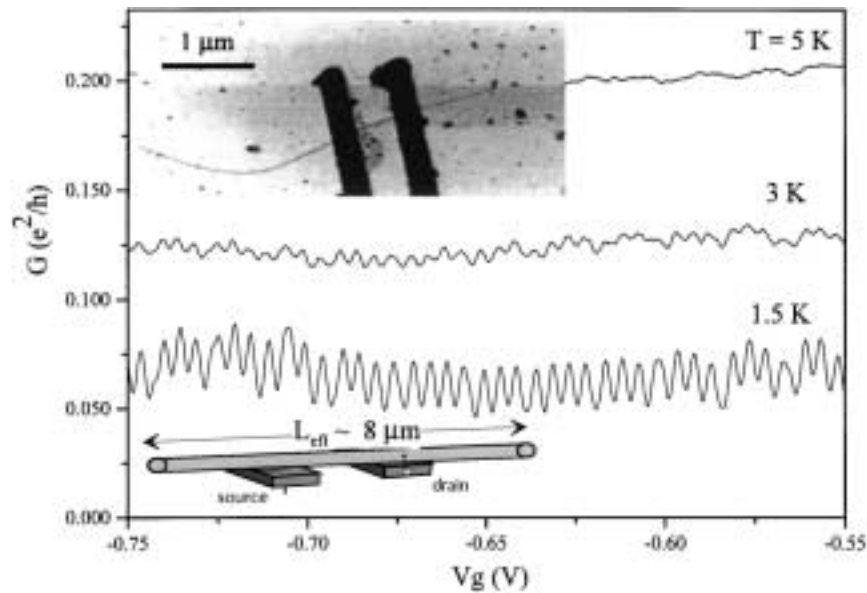
Bachtold *et al.* (Basel) PRL **84** (2000) 6082

J. Kong *et al.* (Stanford) PRL **87** (2001) 106801

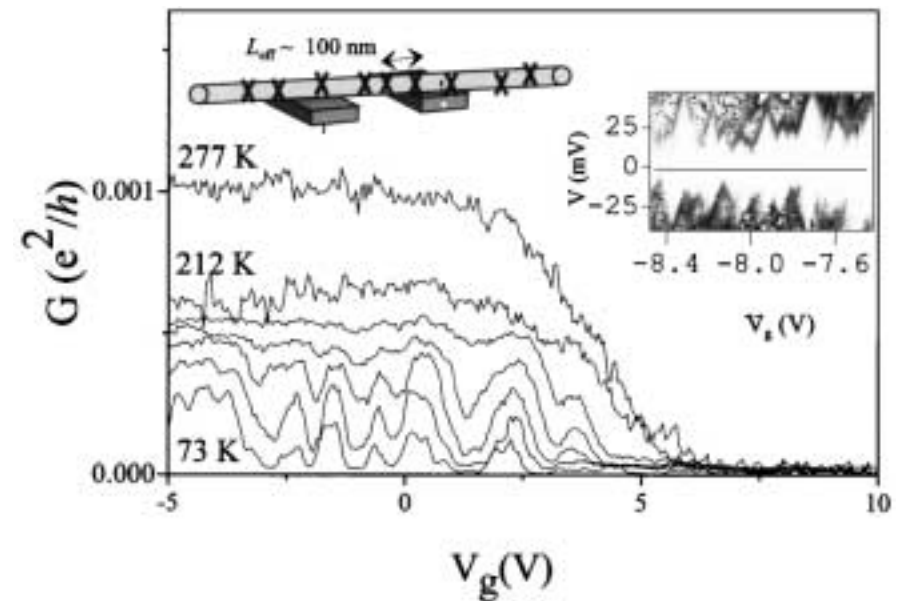
# Experiments

## Coulomb oscillations

**Metallic CN**  
( $L_{eff} \sim 8\mu\text{m}$ )



**Semiconducting CN**  
( $L_{eff} \sim 100\text{nm}$ )



**Single dot**

**Dots in series**

P. L. McEuen *et al.* (Berkeley) PRL **83** (1999) 5098

# Impurity Potential in Carbon Nanotubes

## 1. Metallic CN and Semiconducting CN

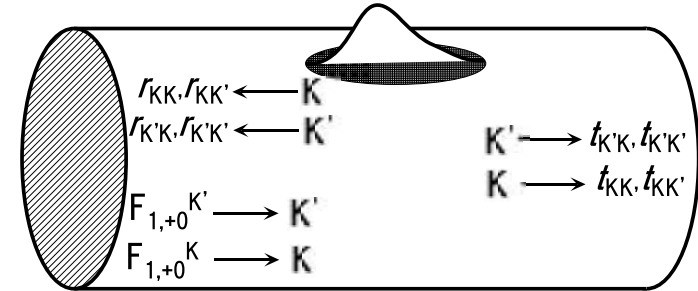
Linear dispersion

## 2. Absence of Back Scattering

(Long-Range Potential)

Ballistic transport, Huge Conductivity

Berry's Phase, Huge Positive Magnetoresistance



What is impurity?

Long-Range: Nano Particle, Metallic Particle, etc.,

Short-Range: Lattice Defects

— Tight-Binding Model —

T. Nakanishi, and T. Ando, J. Phys. Soc. Jpn. **68**,561 (1999)

○Landauer's Formular 
$$G = \frac{2e^2}{h} \sum_{m,n} |t_{mn}|^2,$$

$t_{mn}$  : Transmission Coefficients

$r_{mn}$  : Reflection Coefficients

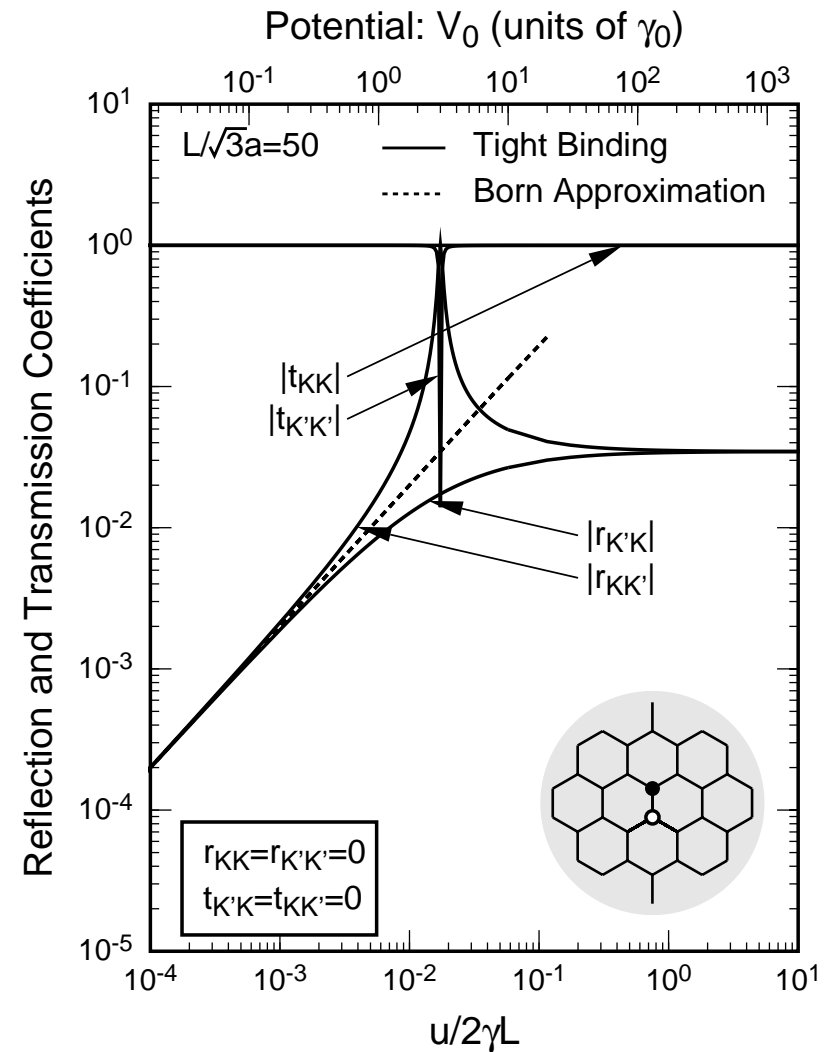
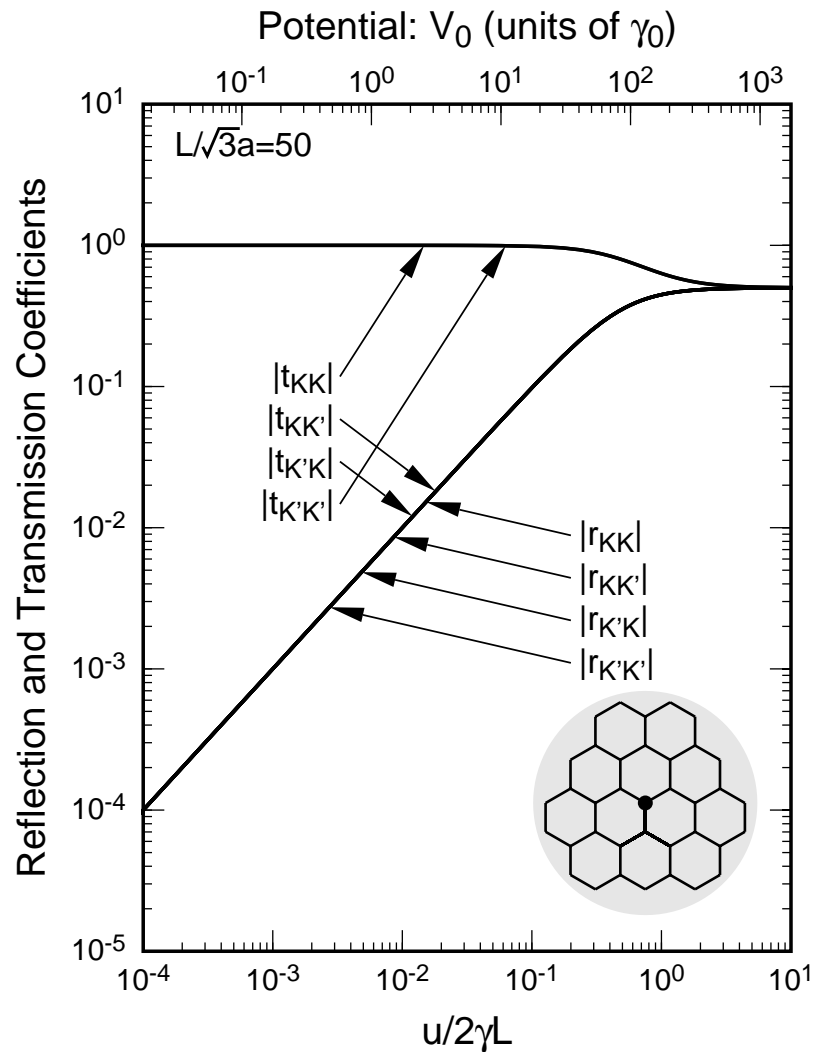
$$\{m, n\} = \{\mathbf{K}, \mathbf{K}\}, \{\mathbf{K}', \mathbf{K}\}, \\ \{\mathbf{K}, \mathbf{K}'\}, \{\mathbf{K}', \mathbf{K}'\}$$

Recursive Green's Function Technique

T. Ando: PRB**42**, 5626 (1990).

# Short Range Potential ( $d/a \rightarrow 0$ )

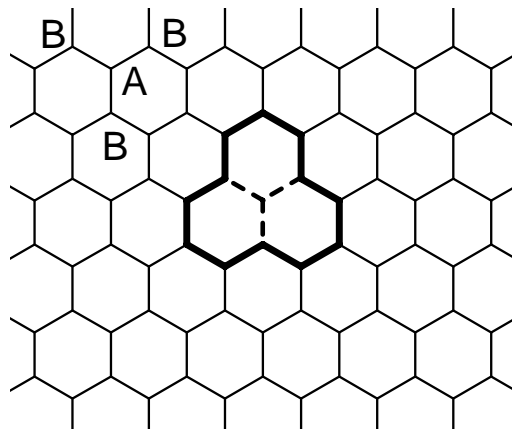
T. Ando, T. Nakanishi, and R. Saito, *Microelectronic Engineering*, 47 (1999) 421



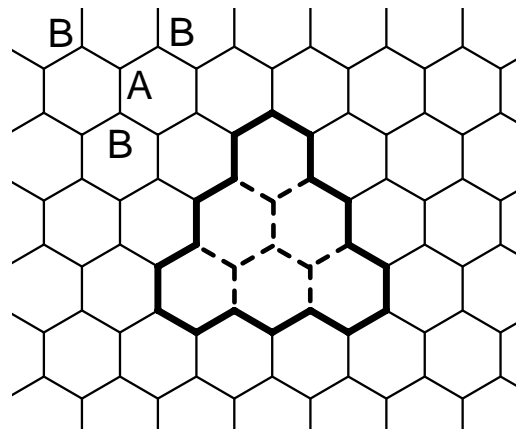
# Lattice Vacancy and Conductance Quantization at $\varepsilon = 0$

M. Igami, T. Nakanishi, and T. Ando, J. Phys. Soc. Jpn. **68**,716 (1999)

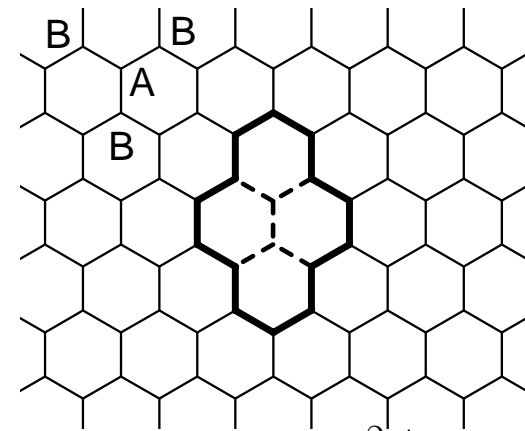
**(a)** Vacancy I



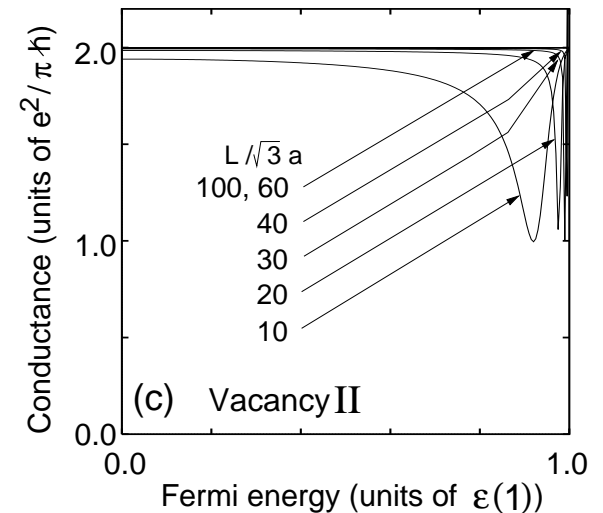
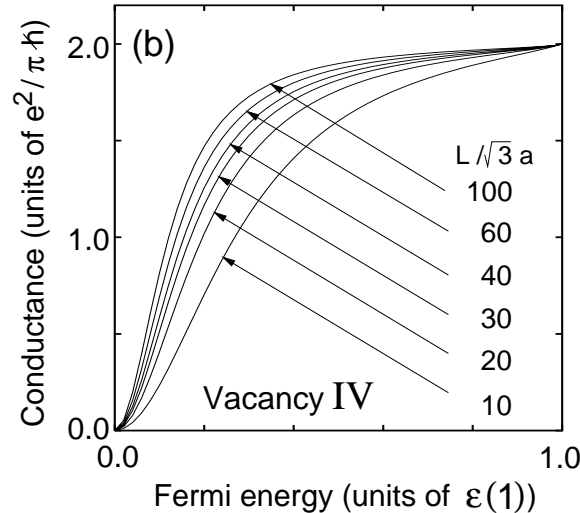
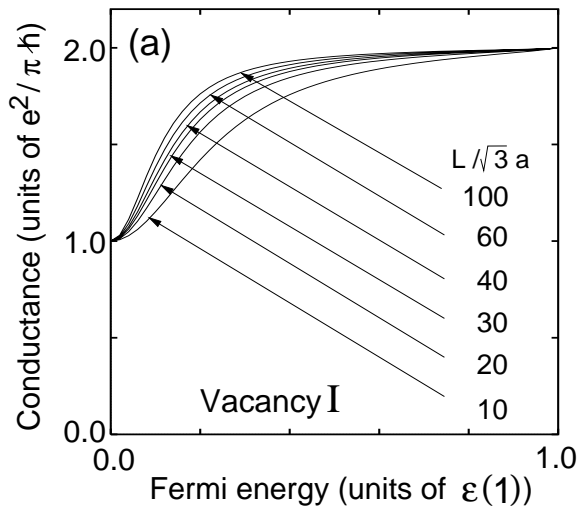
**(b)** Vacancy IV



**(c)** Vacancy II

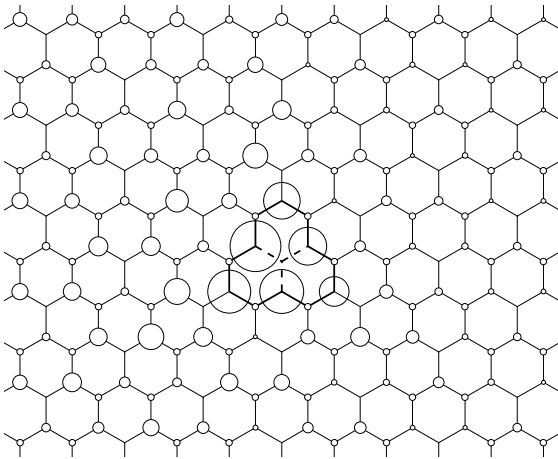


$$G - 2e^2/\pi\hbar \propto 1/L^2$$

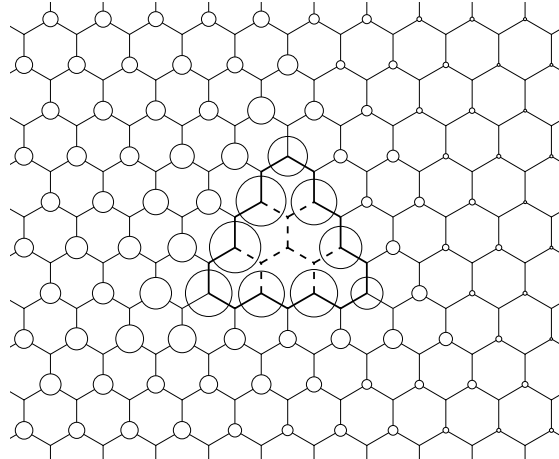


## Wave Functions at $\varepsilon = 0$

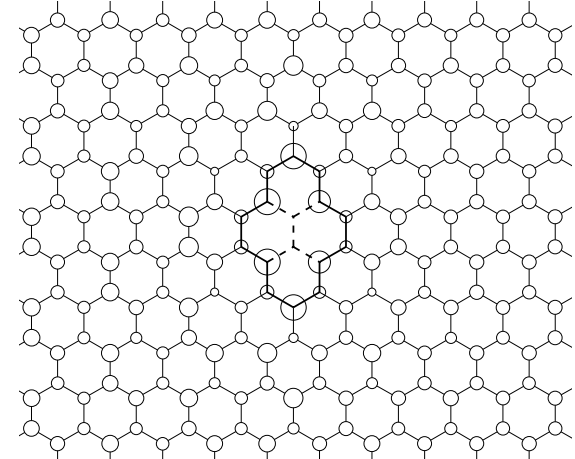
(a) Vacancy I  $\longrightarrow$  Tube axis



(b) Vacancy IV  $\longrightarrow$  Tube axis



(c) Vacancy II  $\longrightarrow$  Tube axis



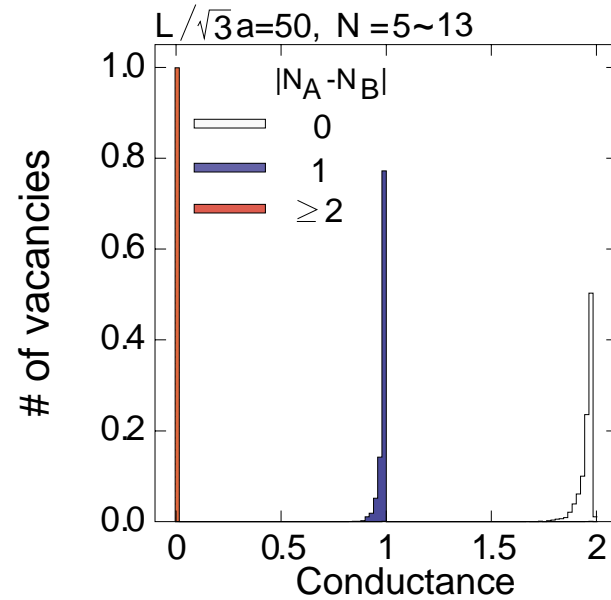
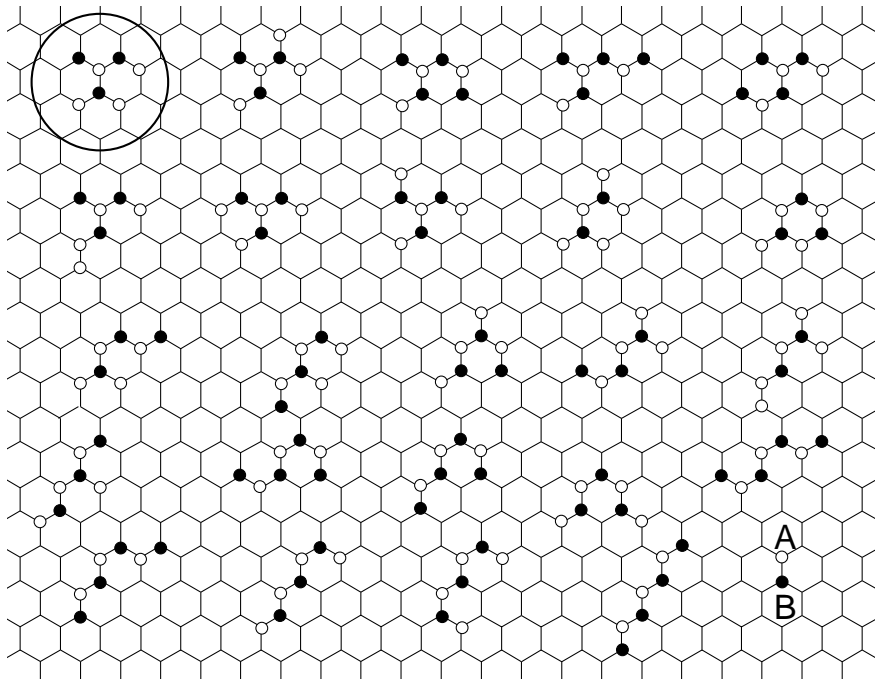
1. Vacancy I: three sublattice Kekulé pattern  
Standing Wave (K and K' point)
2. Vacancy IV: Large amplitude at B sites  
no component on A sites (left-hand side)
3. Vacancy II: not disturbed by the vacancy

# Quantization Rule at $\varepsilon = 0$

M. Igami, T. Nakanishi, and T. Ando, J. Phys. Soc. Jpn. 68 (1999) 3146

Examples for  $N = N_A + N_B = 7$

Tube Axis  $\rightarrow$



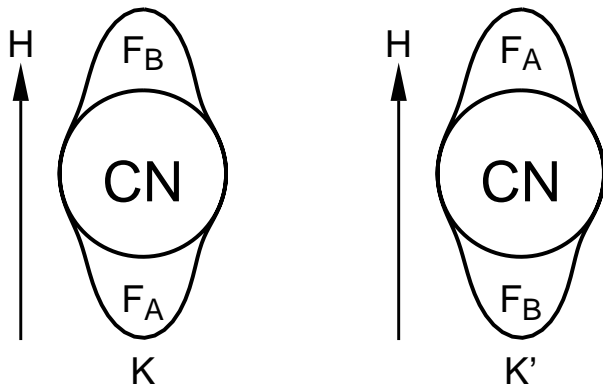
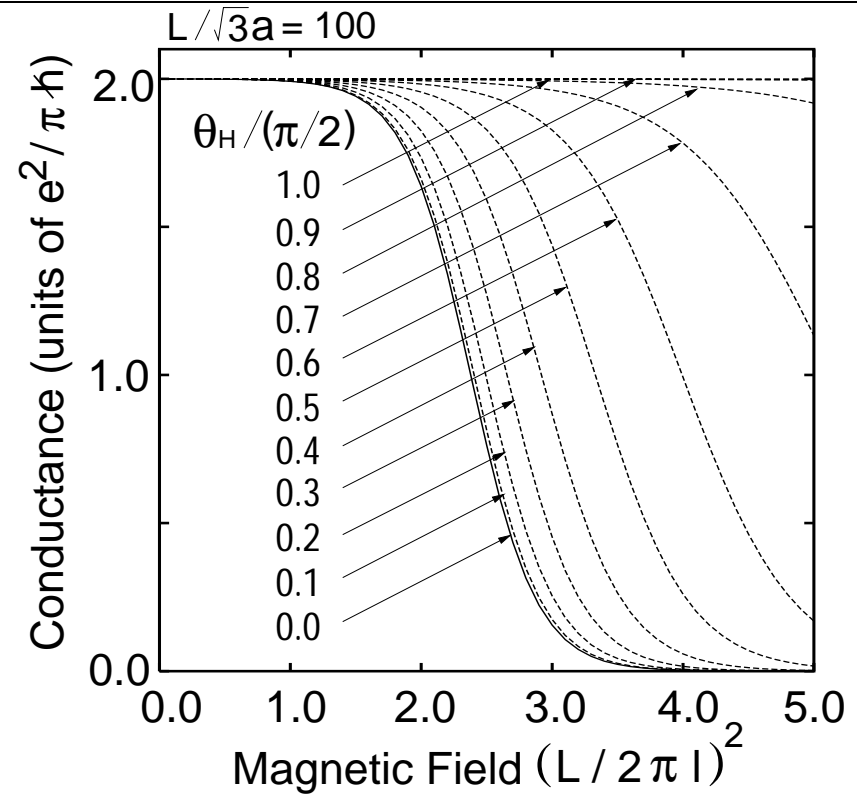
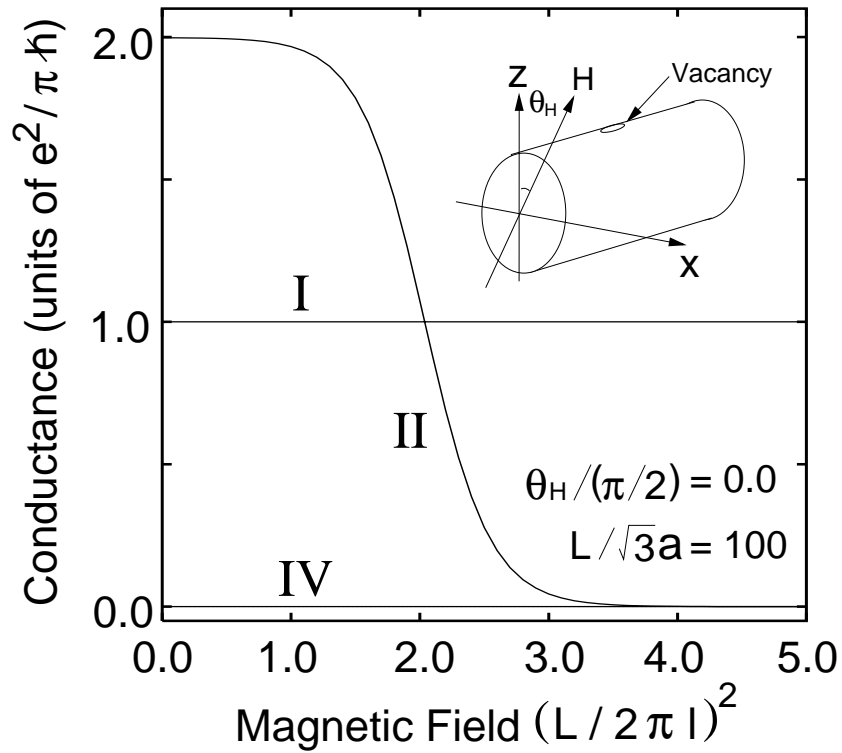
## Quantization Rule at $\varepsilon = 0$

$1.6 \times 10^5$  different CN's with a vacancy

$N_A, N_B$ : number of removed A and B sublattice sites

$ N_A - N_B $	1	The Others ( $\geq 2$ )	0
Conductance	$e^2/\pi\hbar$	0	$\sim 2e^2/\pi\hbar$

# Magnetic Field



**Solid Line: Conductance vs.  $H \cos \theta_H$**

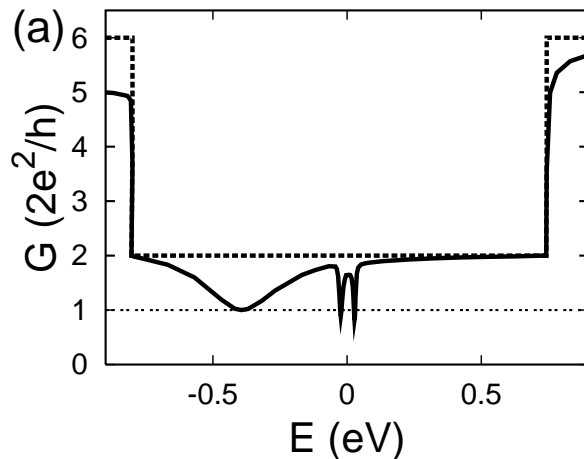
M. Igami, T. Nakanishi, and T. Ando,  
J. Phys. Soc. Jpn. **68**,716 (1999)

# Defects in Carbon Nanotubes

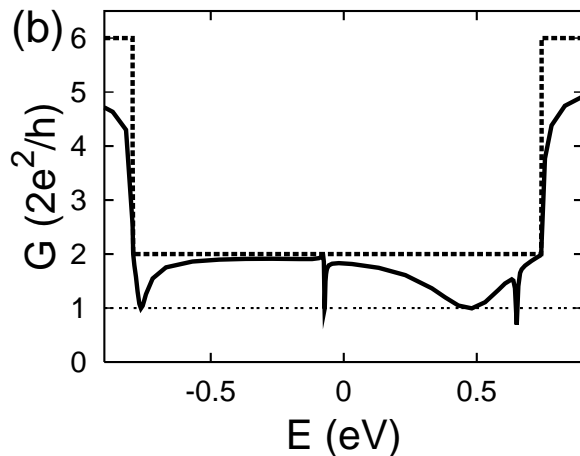
H. J. Choi, *et al.* PRL 84, 2917 (2000)

*ab initio* study on transport in CN with B and N

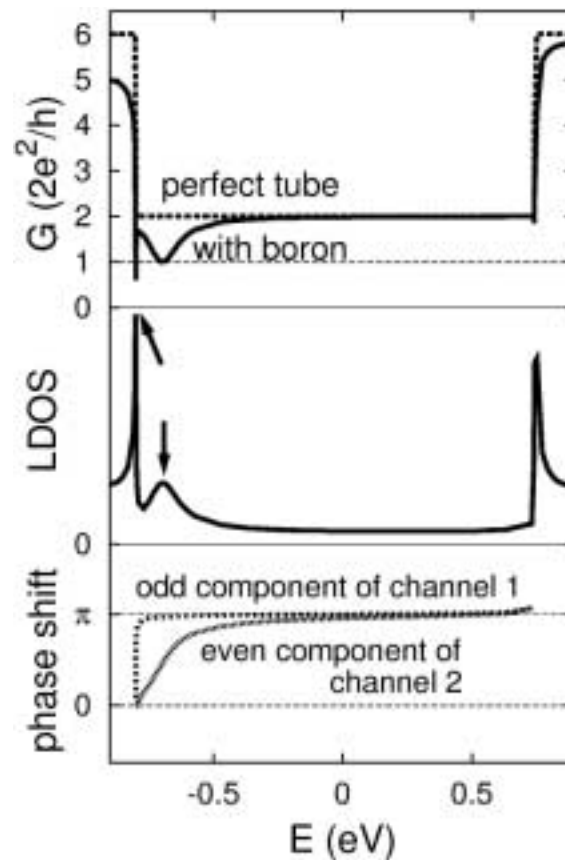
Point vacancy



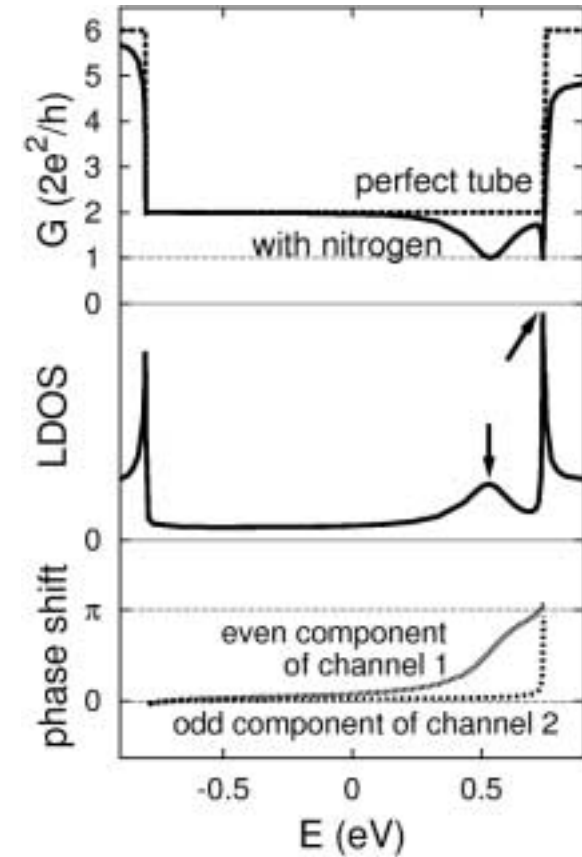
Double vacancy



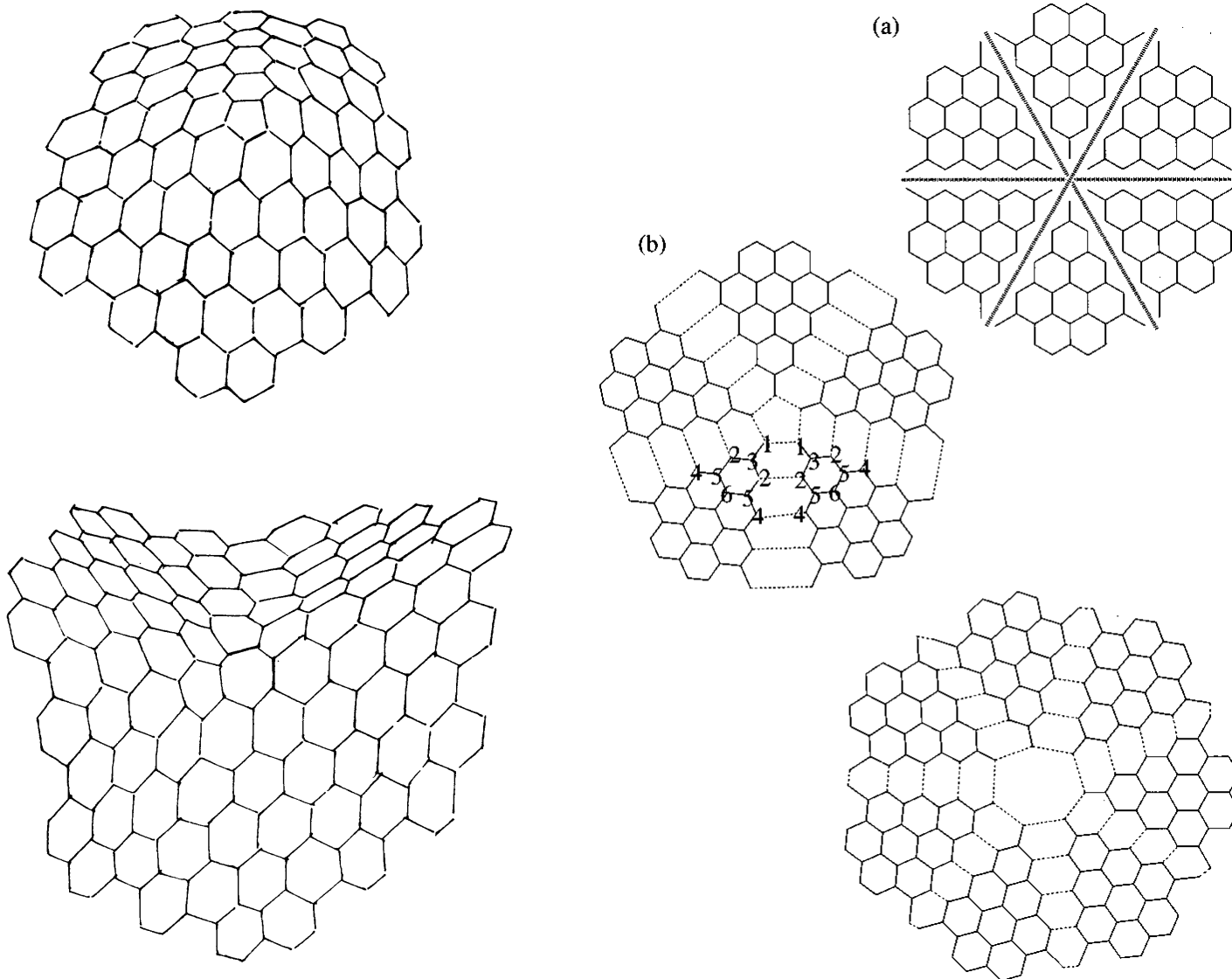
Boron: Acceptor



Nitrogen: Donor

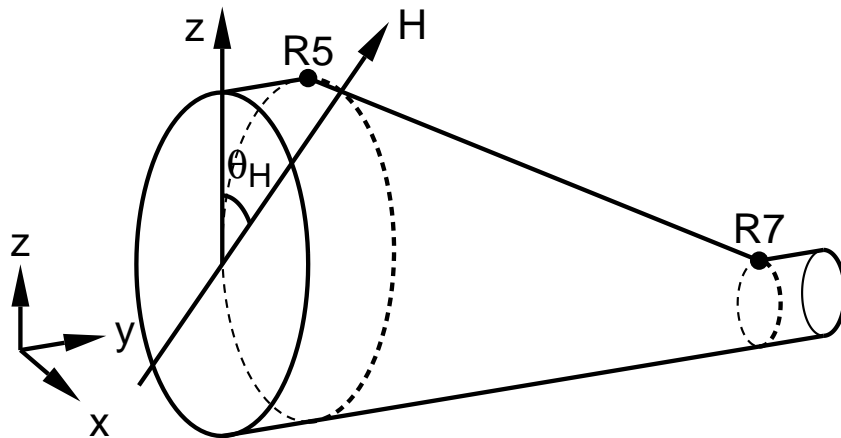
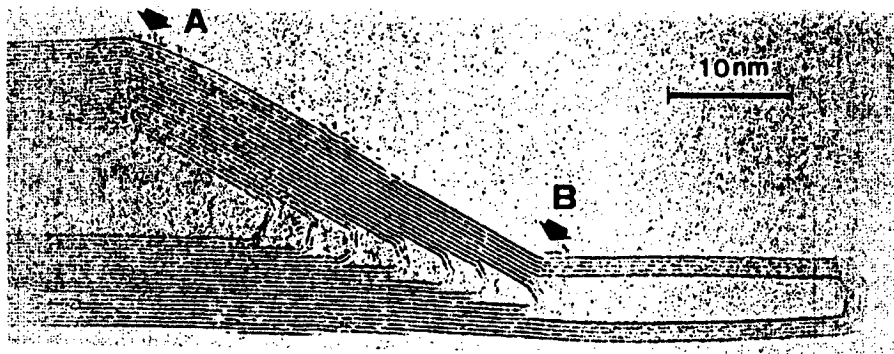


# Topological Defects

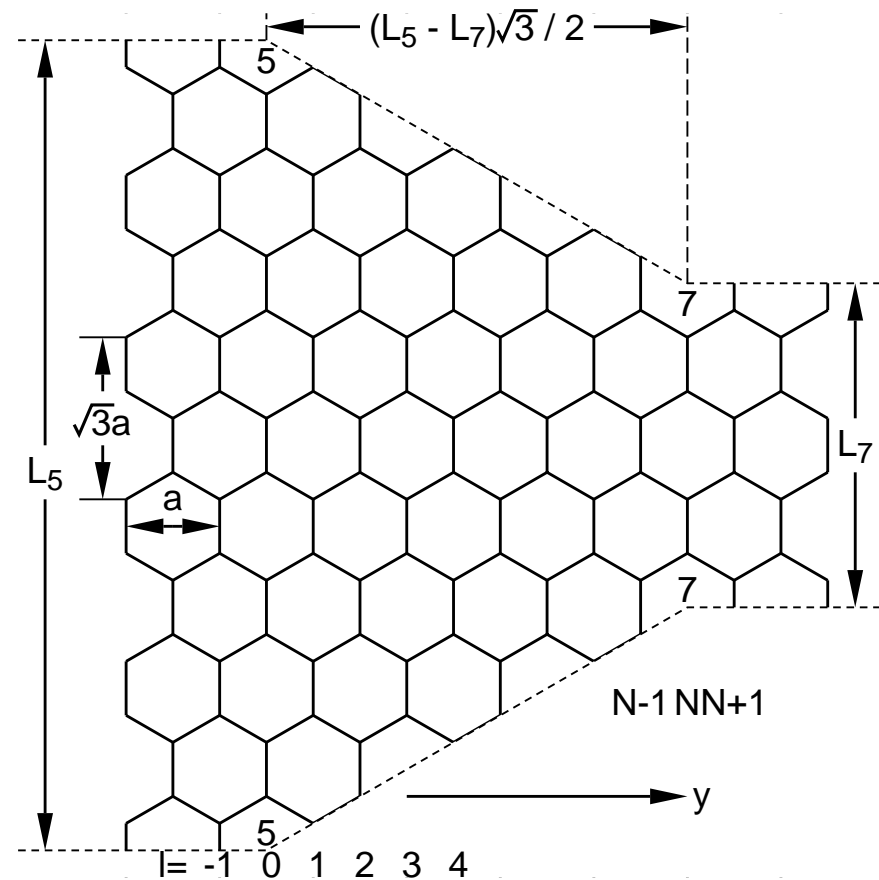


# Carbon Nanotube Junction

S. Iijima, T. Ichihashi and Y. Ando, Nature (London), **356**, 776 (1992).



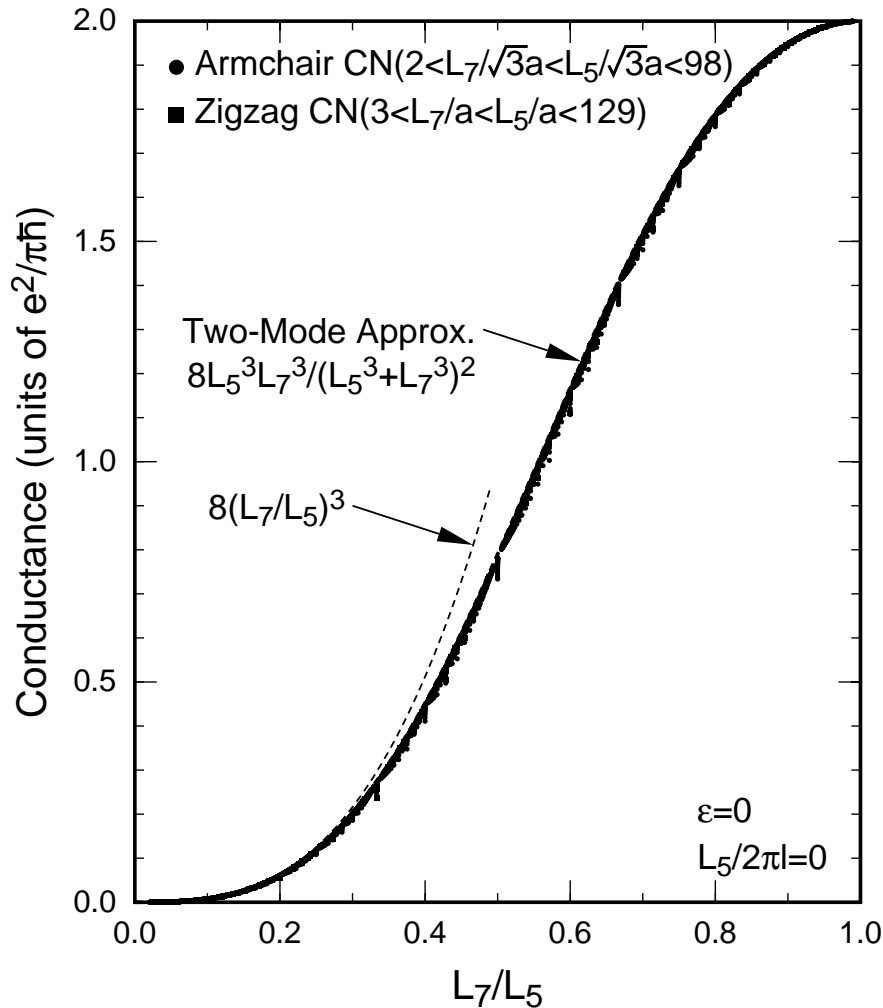
R5 (A): five-membered ring



R7 (B): seven-membered ring

# Conductance of CN Junctions ( $H = 0$ )

R. Tamura and M. Tsukada, PRB55, 4991 (1997).



Conductance exhibits a universal power-law dependence on  $L_7/L_5$

$$G \propto (L_7/L_5)^3 \quad \text{for } L_5 \gg L_7.$$

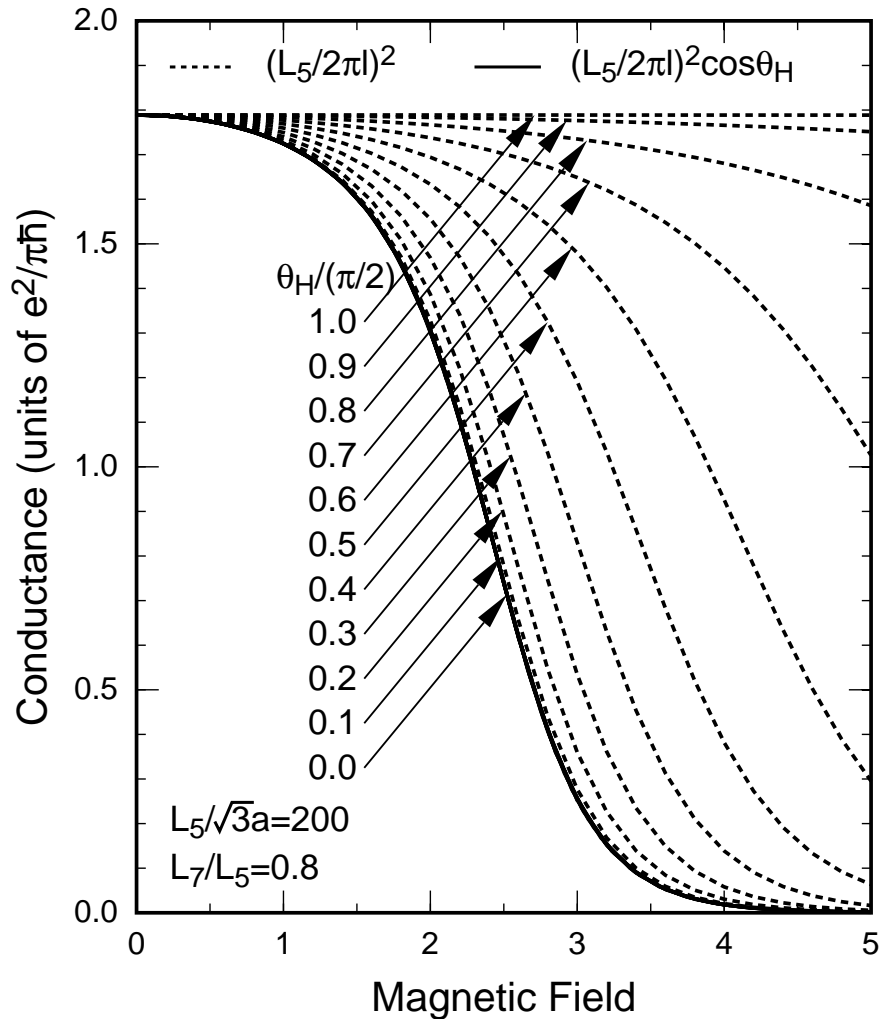
**Effective-Mass Theory**

**Wave function decay linearly**

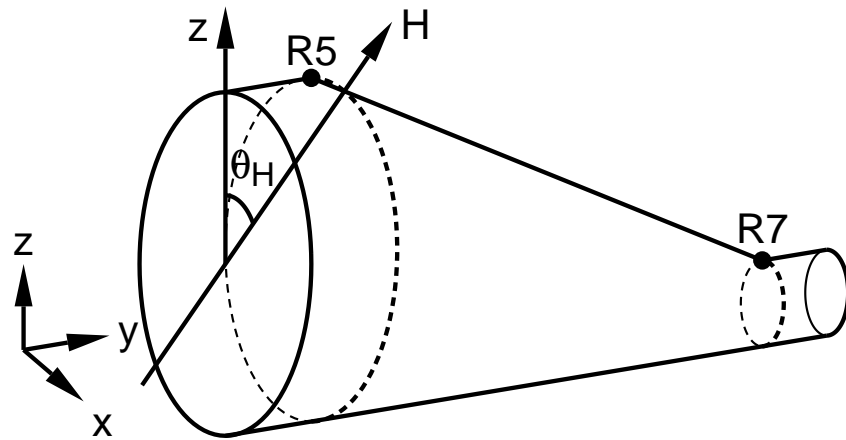
H. Matsumura and T. Ando, J. Phy. Soc. Jpn., **67**,  
 3542 (1998).

# CN Junction with Magnetic Field

T. Nakanishi and T. Ando, J. Phys. Soc. Jpn., **66**, 2973 (1997)



Conductance depends only on  $z$  component of  $H$



Solid Line: Conductance vs.  $H \cos\theta_H$

## Conclusion

### Interesting Electronic Properties of Carbon nanotubes

1. Long quasi-one dimensional system
2. Metallic CN and Semiconducting CN
3. Linear dispersion
4. Neutrinos on cylinder surface

#### Collaborators

Tsuneya Ando (ISSP→TIT)

Masatsura Igami (NISTEP)

Riichiro Saito (Tohoku Univ.)

### Quantum transport in Carbon Nanotubes

1. Absence of Back Scattering for Long-Range Potential  
Ballistic transport, Huge conductivity, Quantized conductance,  
Berry's phase,  
Huge positive magnetoresistance
2. Lattice Vacancy  
Conductance quantization, Donor and acceptor
3. Carbon Nanotube Junctions