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
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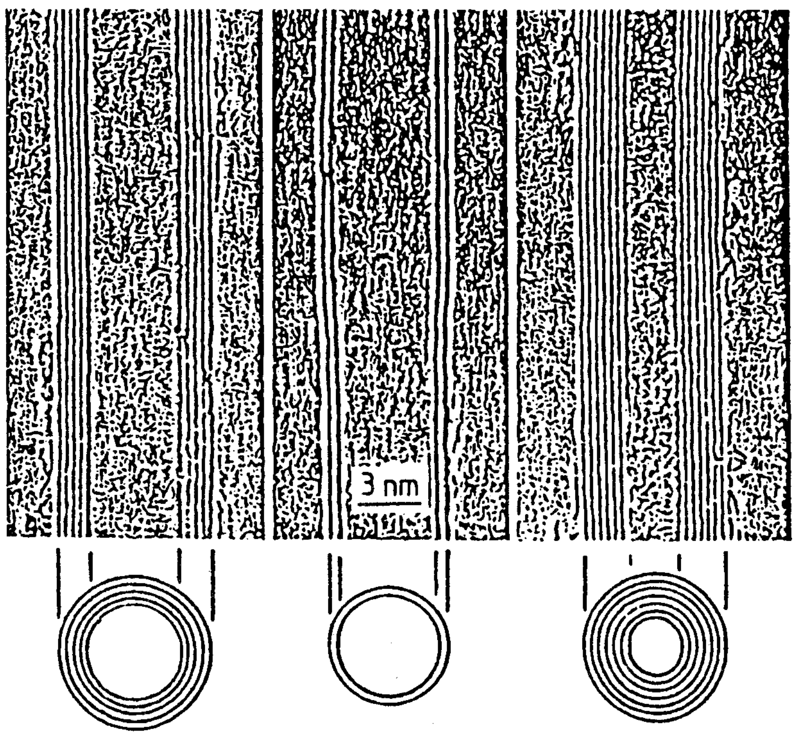
Carbon Nanotubes

Multi-wall

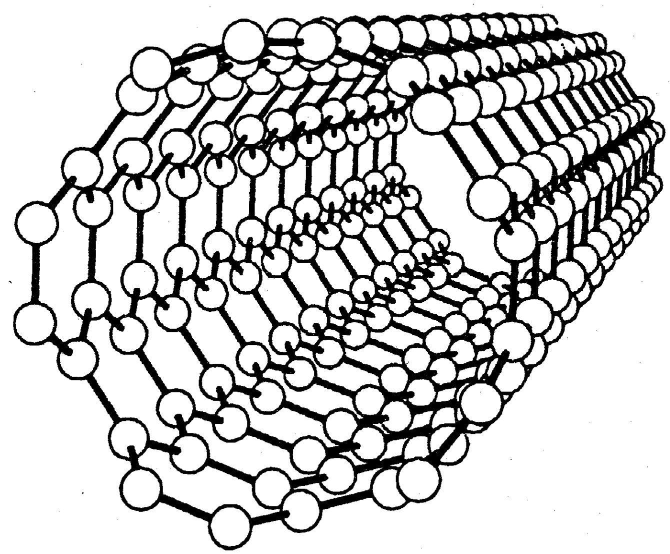


Electron micrographs of CN

S. Iijima, Nature 354, 56 (1991)

Length $\sim 1\mu m$
Diameter $2 \sim 30$**nm**

Single-wall

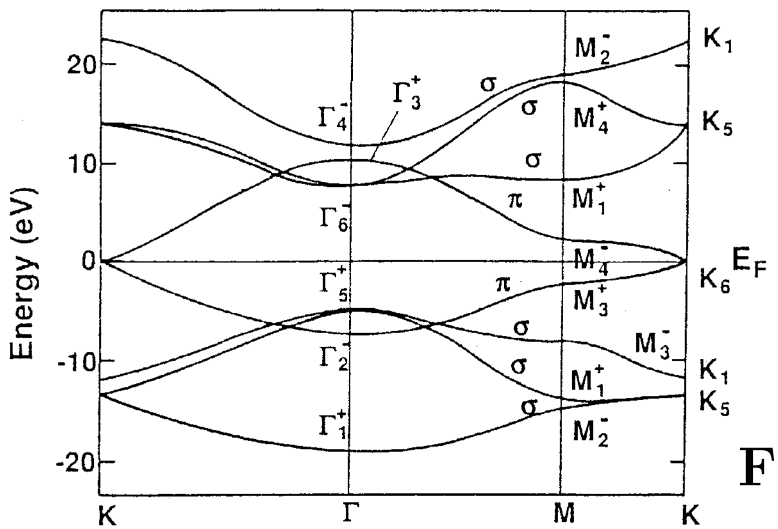


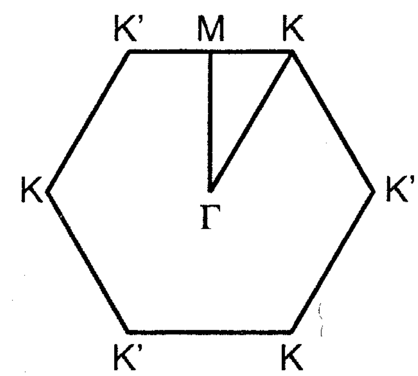
Quantum wire growing naturally

Diameter ~ 4 **nm**
1D level spacing ~ 0.8 **eV**

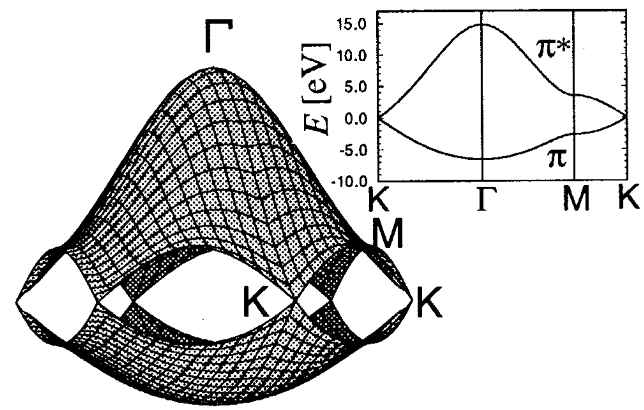
○ **Graphene with periodic boundary condition**

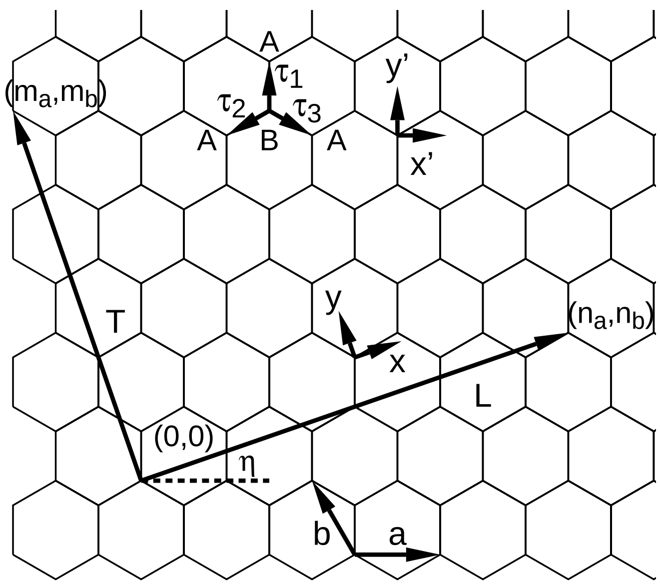
Graphite sheet (Graphene)





First Brillouin Zone





sp^2 covalent bonding

single π band

tight–binding model

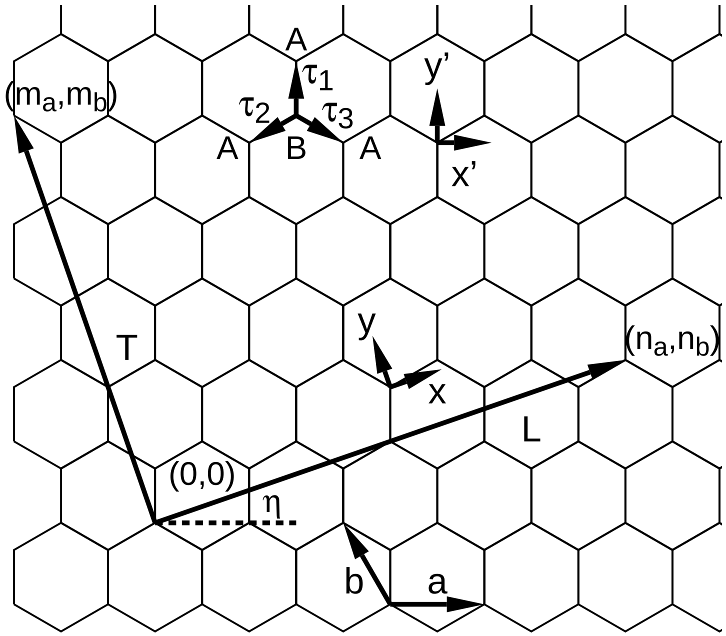
Nearest–neighbor

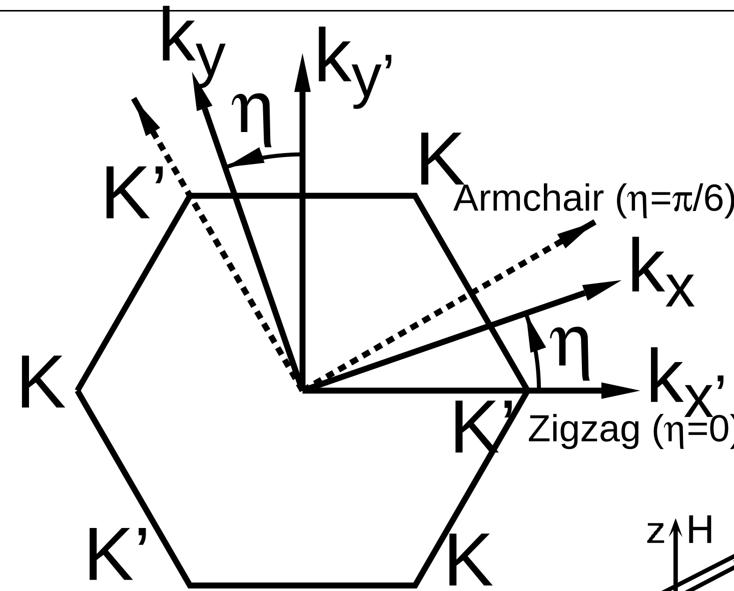
Transfer Integral: γ_0

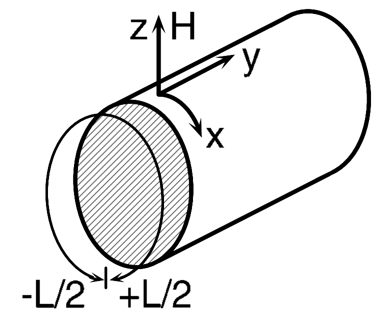
$$-\gamma_0 \sum_{l=1}^{3} \psi_B(\mathbf{R}_A - \vec{\tau}_l) \;=\; \varepsilon\psi_A(\mathbf{R}_A),$$

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

Graphite and Chiral Vector





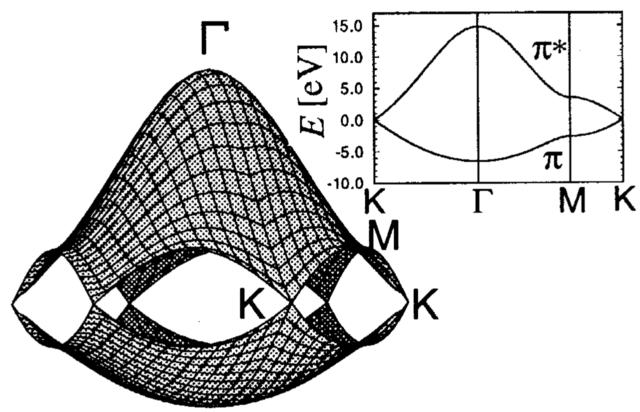


$$\textbf{Chiral Vector:}\mathbf{L} \;=\; n_a\mathbf{a} + n_b\mathbf{b} \equiv (n_a, n_b),$$

$$L = |\mathbf{L}| \;=\; a\sqrt{{n_a}^2 + {n_b}^2 - n_a n_b}.$$

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

$(n_a, n_b) = (1,0)m :$ **zigzag CN**

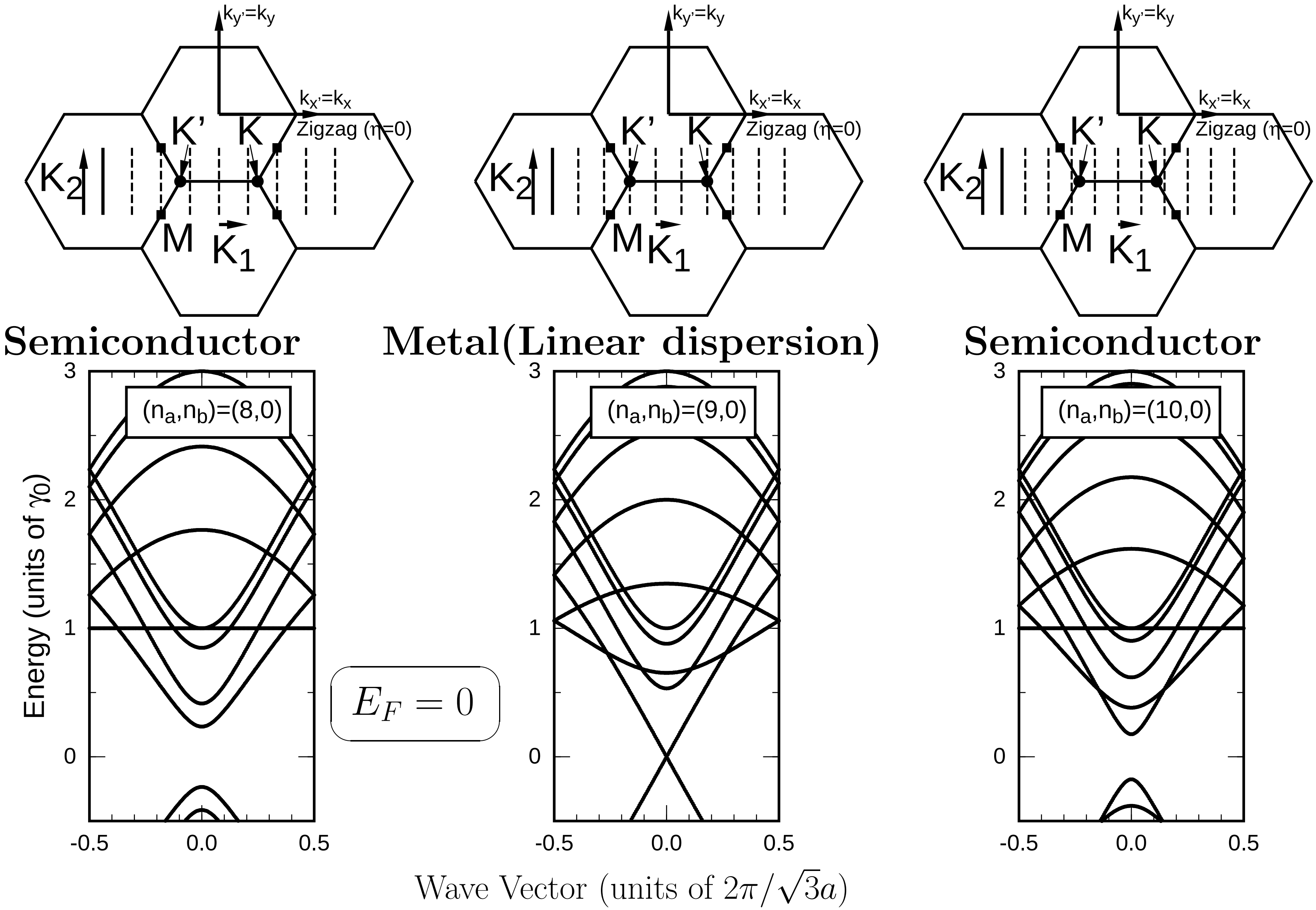


$$n_a + n_b = 3N + \nu$$

$\nu \;=\; 0$ **metallic CN**

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

Metallic and Semiconducting CN (Zigzag CN)



Effective-mass scheme

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

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

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

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

tight–binding model

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

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

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: $\gamma_0 \sim 2.6[\mathbf{eV}]$

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

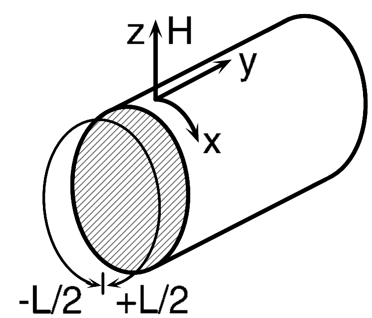
Envelope Function: $\mathbf{F}_K(r)$

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

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

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

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

with

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

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

Energy levels

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

Discritized 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**

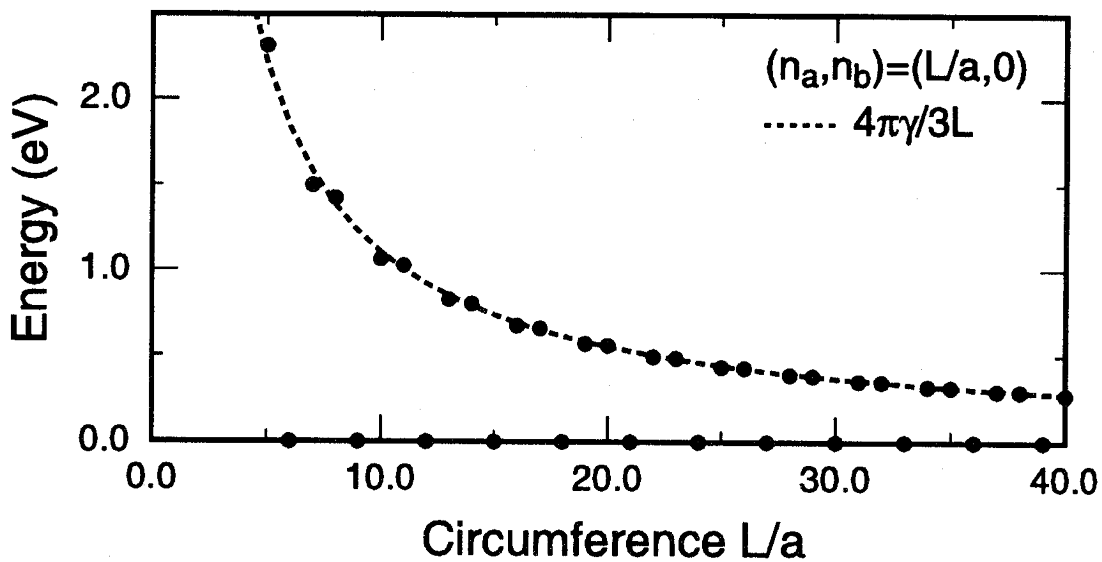
Band gap

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

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

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

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

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

$\mathbf{r}_0$: Impurity Position

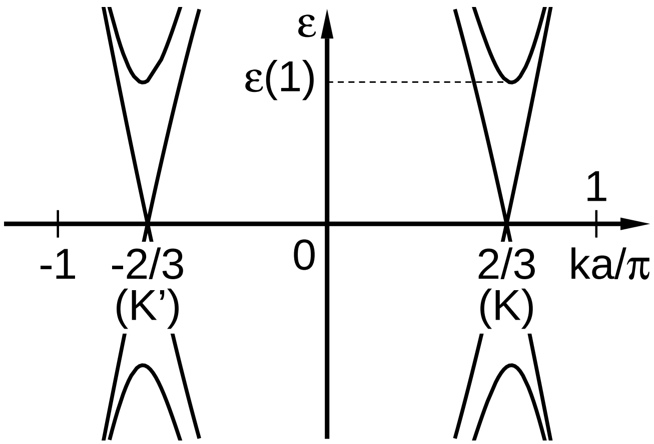
Slowly-varying Potential

Potential Range $d \gg a$

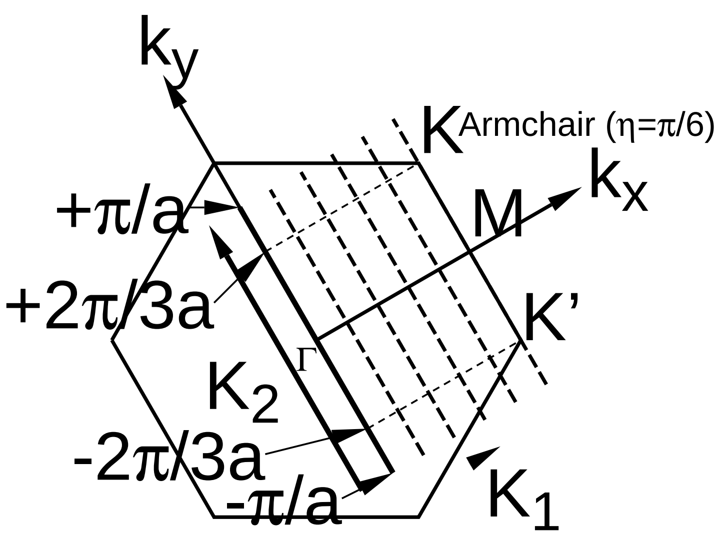
$u_A(\mathbf{r}) = u_B(\mathbf{r})$

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

Right- and left-going channels



Metallic CN



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

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

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

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

A**: Length of Nanotube**
Energy: $\varepsilon(k) = \pm\gamma k$
Group Velocity: $v = \pm\gamma/\hbar$

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

Lowest Born Approximation

◯ Inter-valley Scattering

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

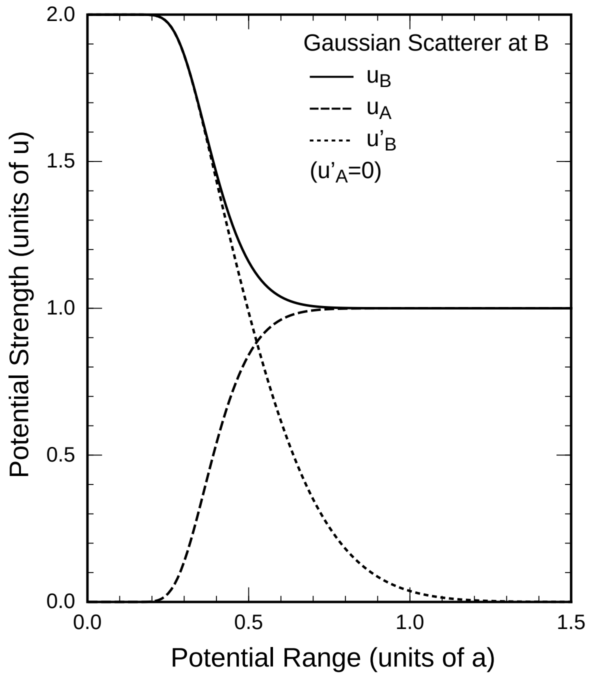
◯ Intra-valley Scattering

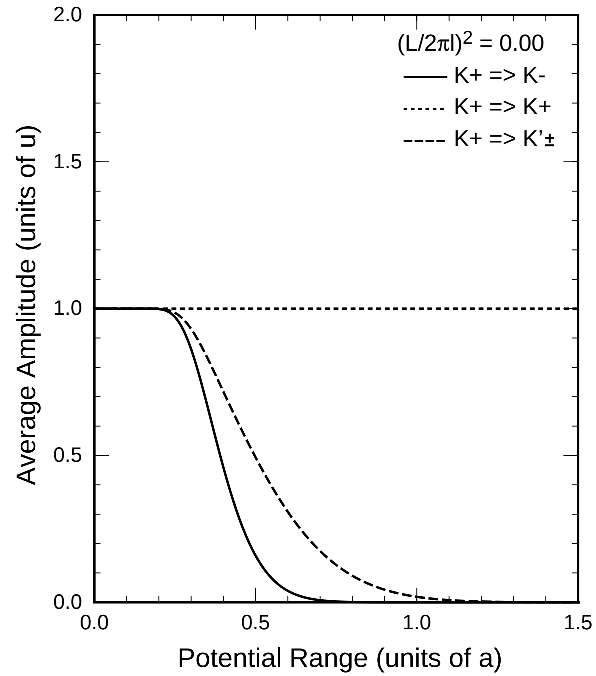
$$\begin{aligned} V_{K\pm K+} &= \frac{1}{2AL}\int d\mathbf{r} \begin{pmatrix} \pm i & 1 \end{pmatrix} \begin{pmatrix} u_A(\mathbf{r}) & 0 \\ 0 & u_B(\mathbf{r}) \end{pmatrix} \begin{pmatrix} -i \\ 1 \end{pmatrix} \\ &= \frac{1}{2AL}\int d\mathbf{r} \left\{ \pm u_A(\mathbf{r}) + u_B(\mathbf{r}) \right\}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

Absence of back-scattering for slowly varying potential

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

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**

$\Downarrow$

Huge Conductivity, Quantized Conductance

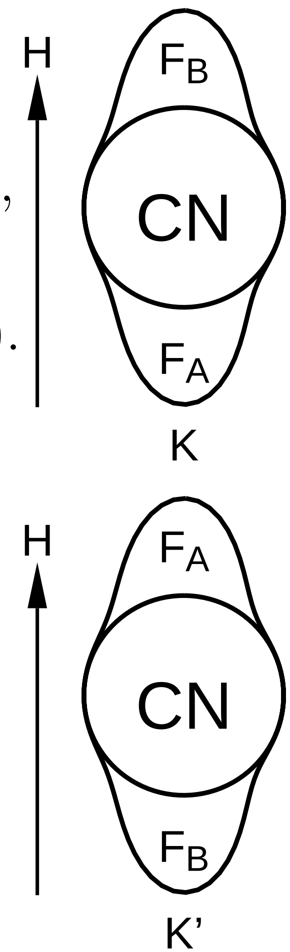
Magnetic Field

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

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

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

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



$$F_{\pm}(x) = \frac{1}{\sqrt{L I_0(\alpha)}} \exp\left[\pm \frac{1}{2} \alpha \cos \frac{2\pi x}{L}\right]$$

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

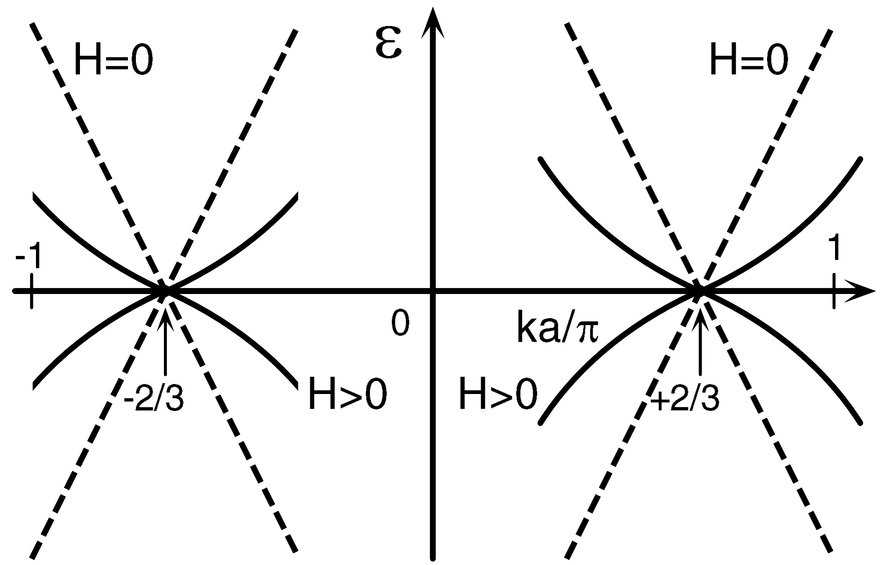
Energy

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

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

Dashed lines: $H = 0$

Solid lines: $H \neq 0$



Lowest Born Approximation

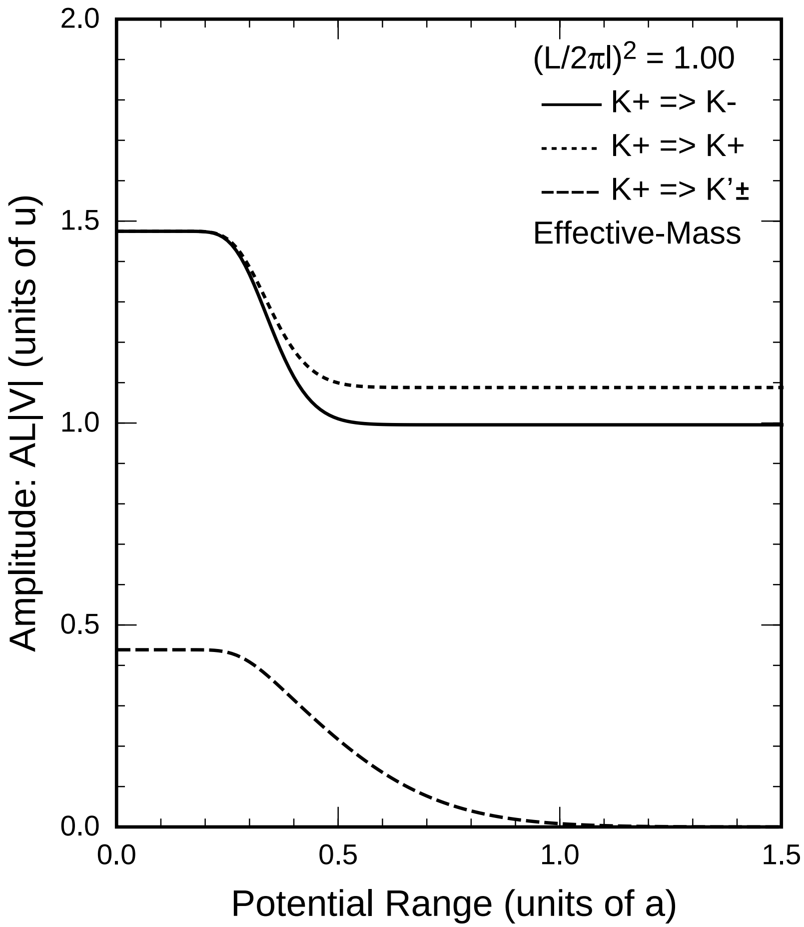
○ **Inter-valley Scattering**

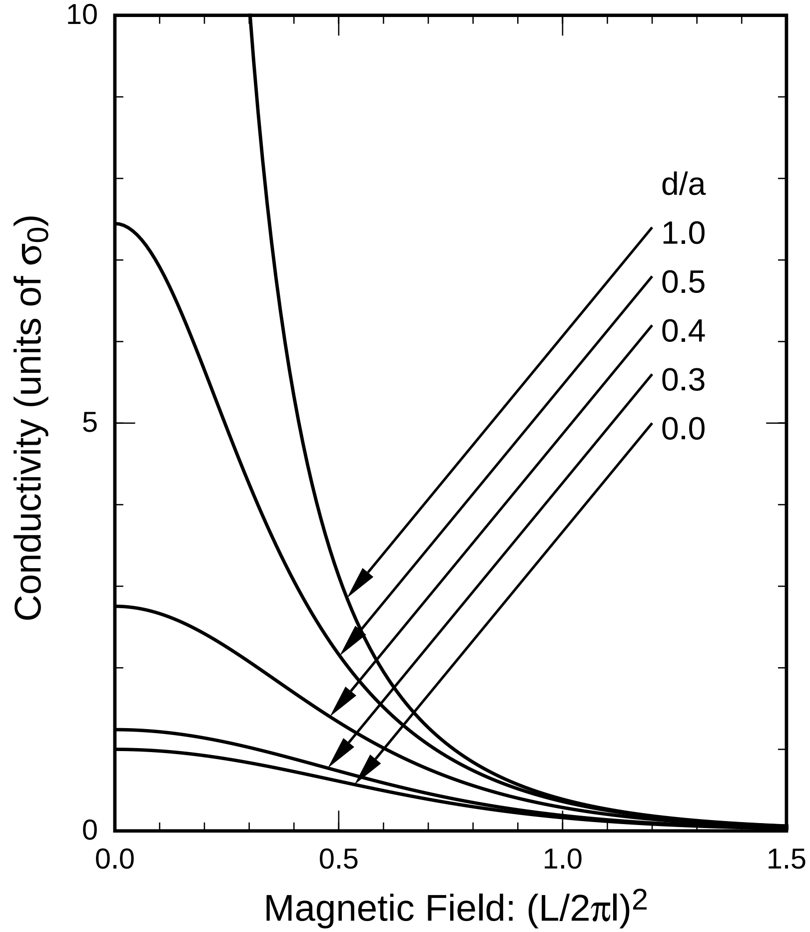
$$V_{K\pm K'+} = \frac{1}{2A}(\mp u'_A e^{i\eta} - \omega^{-1} e^{-i\eta} u'_B) F_+(x_0) F_-(x_0) = V^*_{K'\pm K+}$$

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

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

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

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

Long range Potential

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

$$\begin{aligned} \mathbf{F}_{s\mathbf{k}}(\mathbf{r}) &= \frac{1}{\sqrt{LA}} \exp(i\mathbf{k}\cdot\mathbf{r})\,\mathbf{F}_{s\mathbf{k}}, \\ \varepsilon_s(\mathbf{k}) &= s\gamma|\mathbf{k}|, \\ s &= +1 \quad \textbf{conduction band} \\ s &= -1 \quad \textbf{valence band} \end{aligned}$$

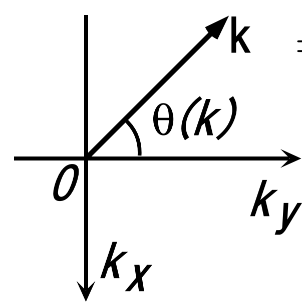
$$\varepsilon_s(-\mathbf{k}) = \varepsilon_s(\mathbf{k})$$

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

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

Spin-rotation operator

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



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

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

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

$(p+1)$th order term

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

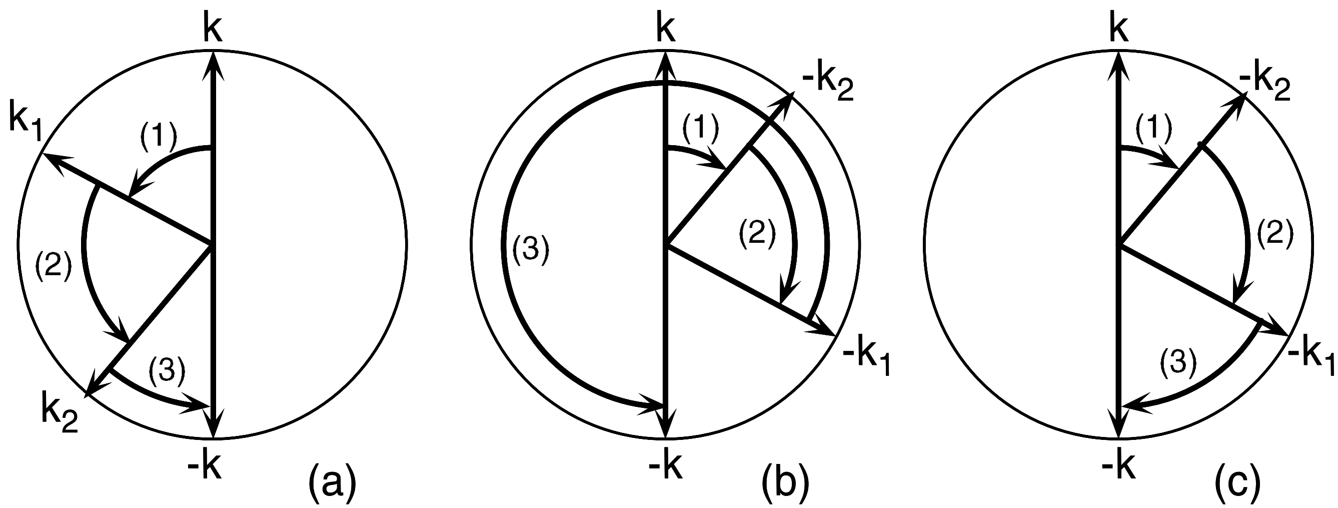
time-reversal terms cancel out

$(s_1,k_1)\rightarrow(s_p,-k_p)$,

$(s_2,k_2)\rightarrow(s_{p-1},-k_{p-1}),\ldots$

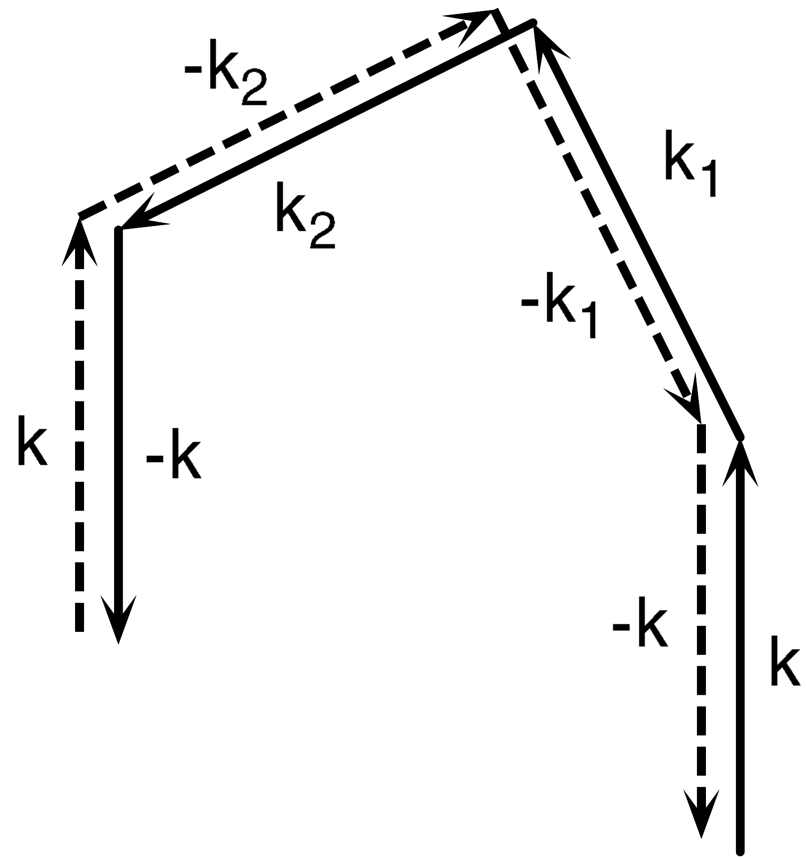
$R[\theta]=-R[\theta+2\pi]$

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



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

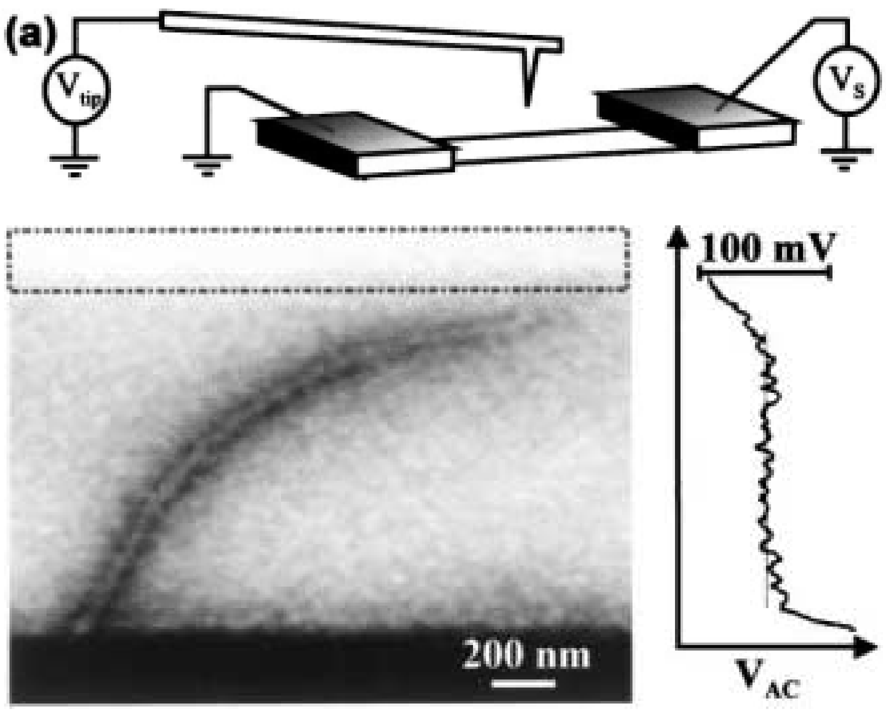
$$\varphi = -i\int_0^T dt\,\left\langle \psi_s[\mathbf{k}(t)] \middle| \frac{d}{dt}\,\psi_s[\mathbf{k}(t)] \right\rangle = \pi$$

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

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

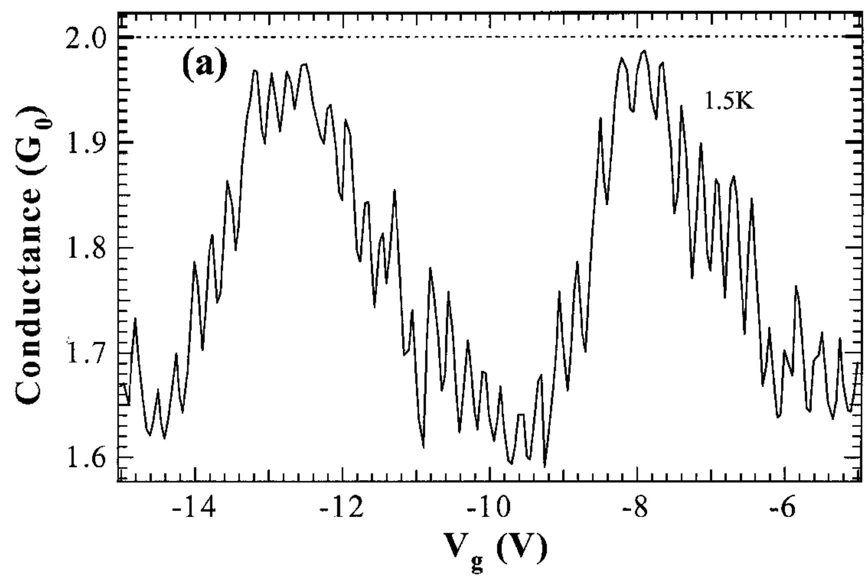
Experiments

0 Voltage Drop



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

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

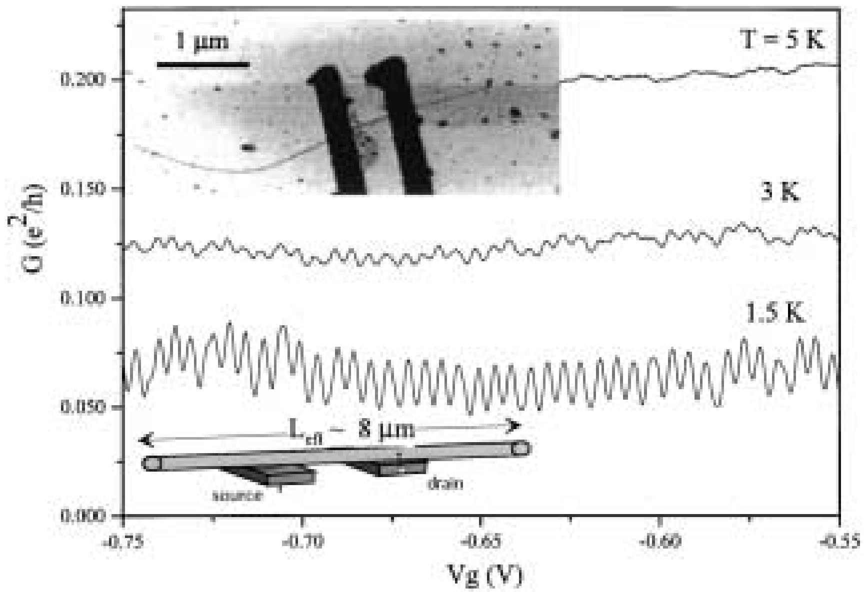


J. Kong *et al*. (Stanford) PRL **87** (2001) 106801

Experiments

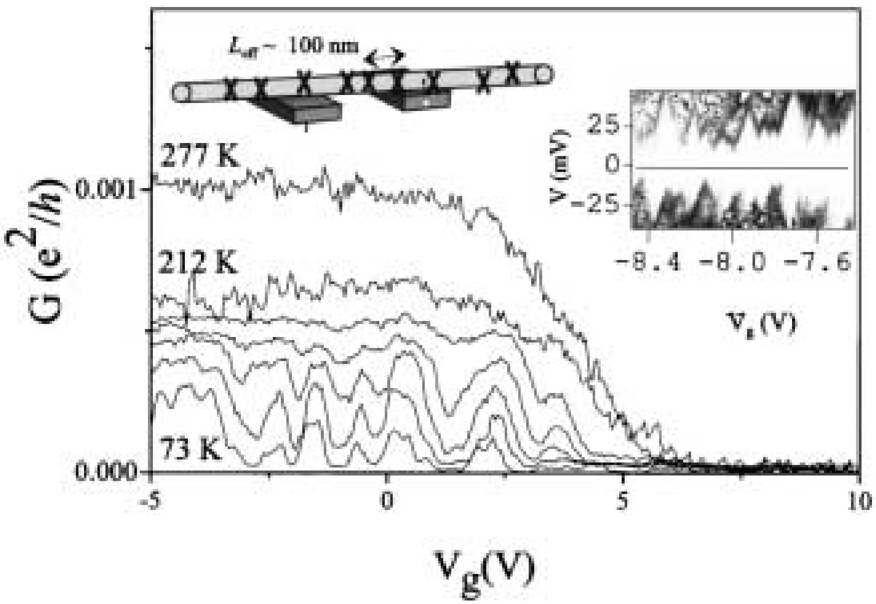
Coulomb oscillations

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



Single dot

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

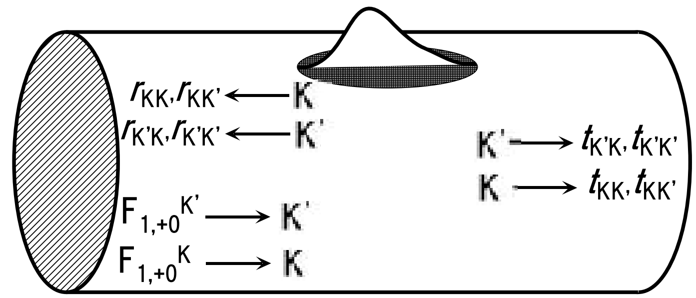


Dots in series

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

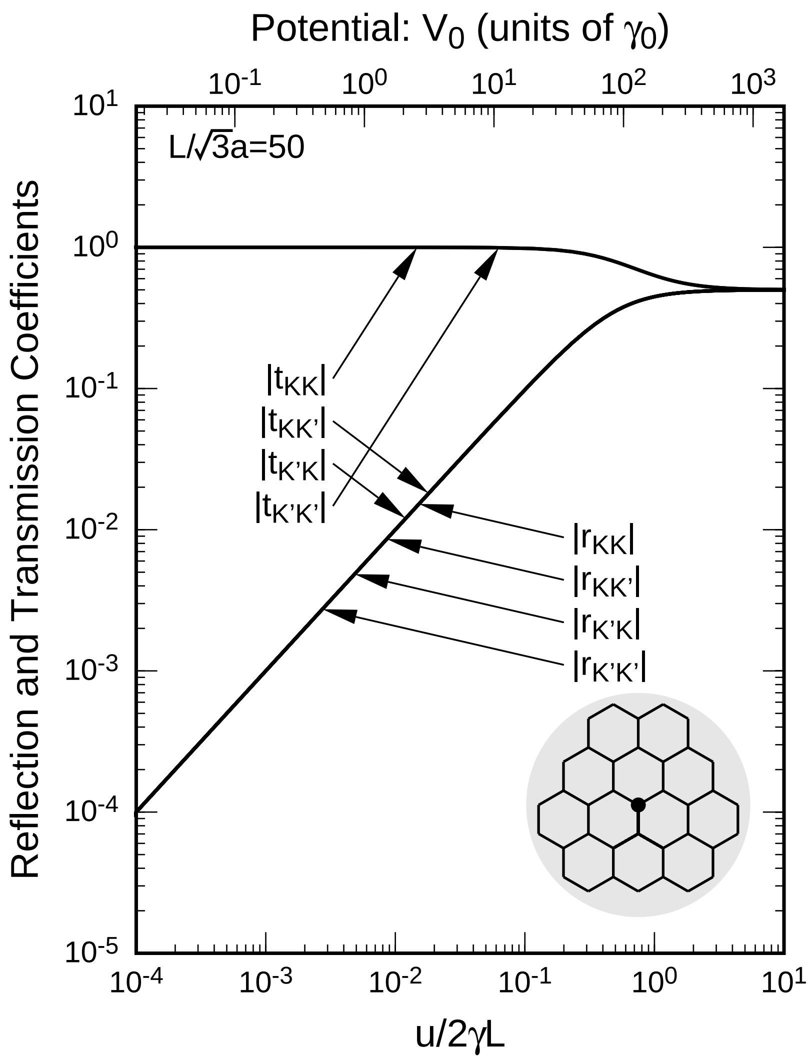
r_{mn} : Reflection Coefficients

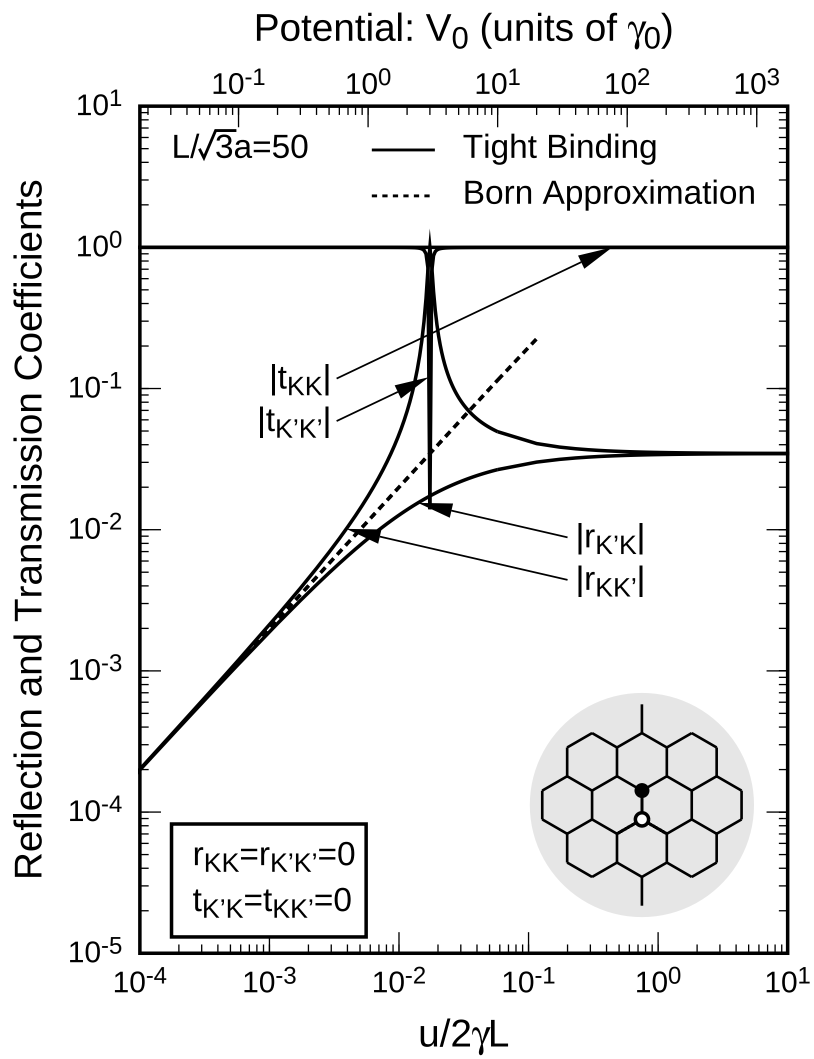
$\{m, n\} = \{\mathbf{K}, \mathbf{K}\}, \{\mathbf{K}', \mathbf{K}\}, \{\mathbf{K}, \mathbf{K}'\}, \{\mathbf{K}', \mathbf{K}'\}$

Recursive Green's Function Technique — T. Ando: PR**B42**, 5626 (1990).

Short Range Potential ($d/a \to 0$)

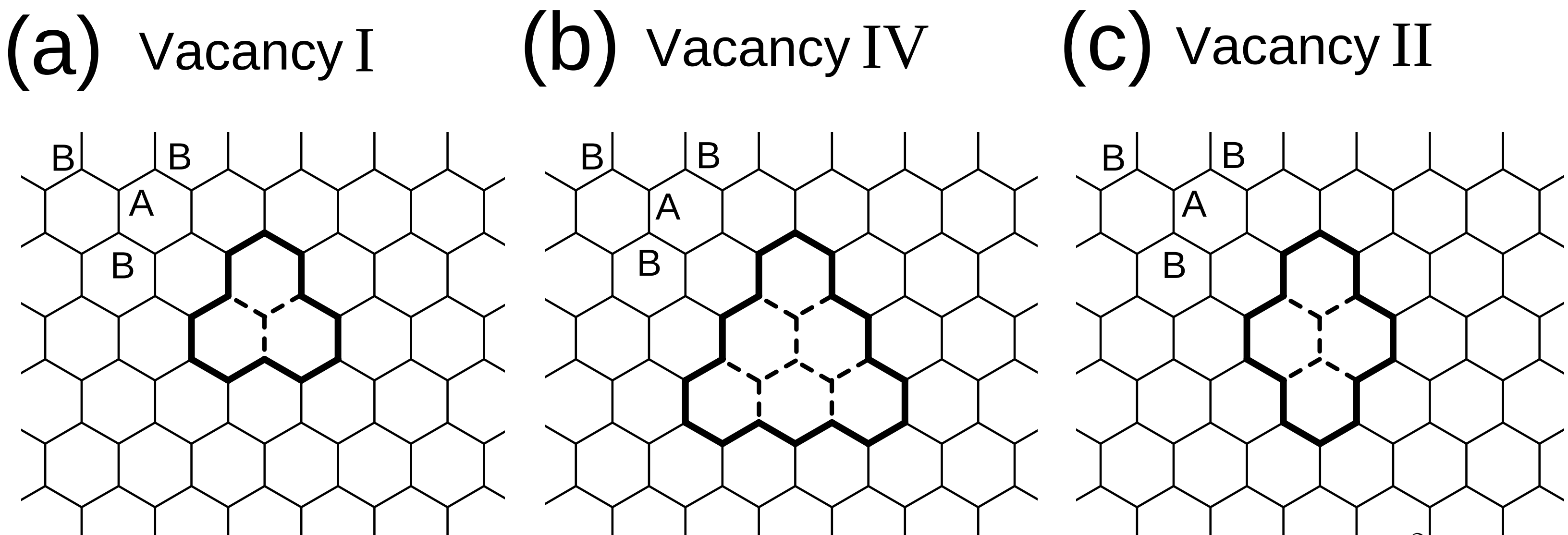
T. Ando, T. Nakanishi, and R. Saito, Microelectronic Engineering, 47 (1999) 421



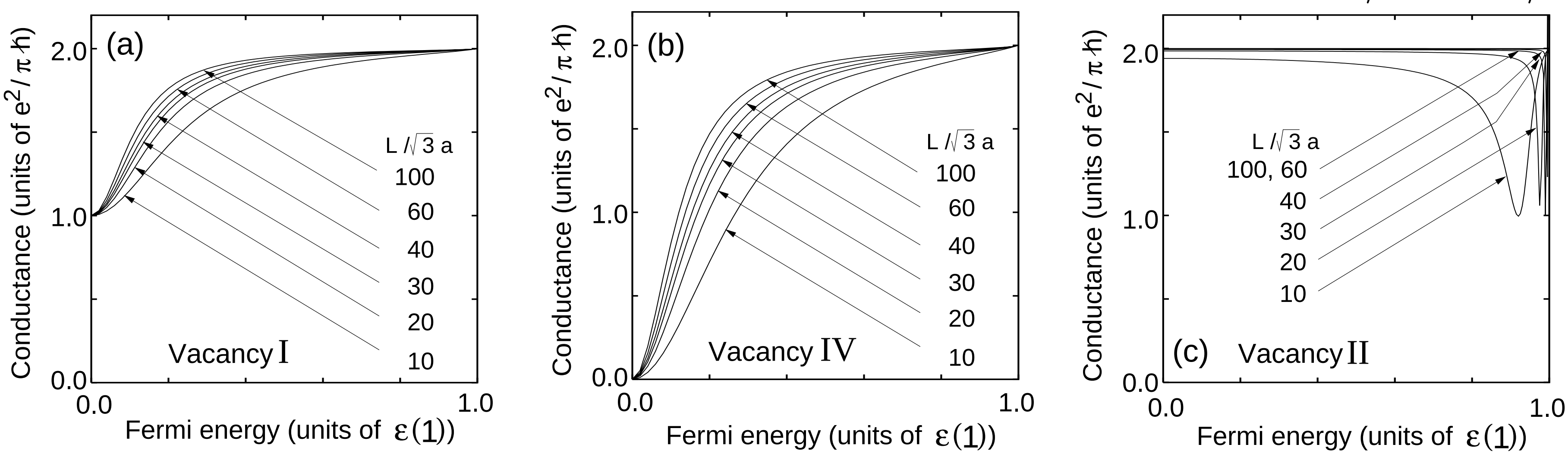


Lattice Vacancy and Conductance Quantization at $\varepsilon = 0$

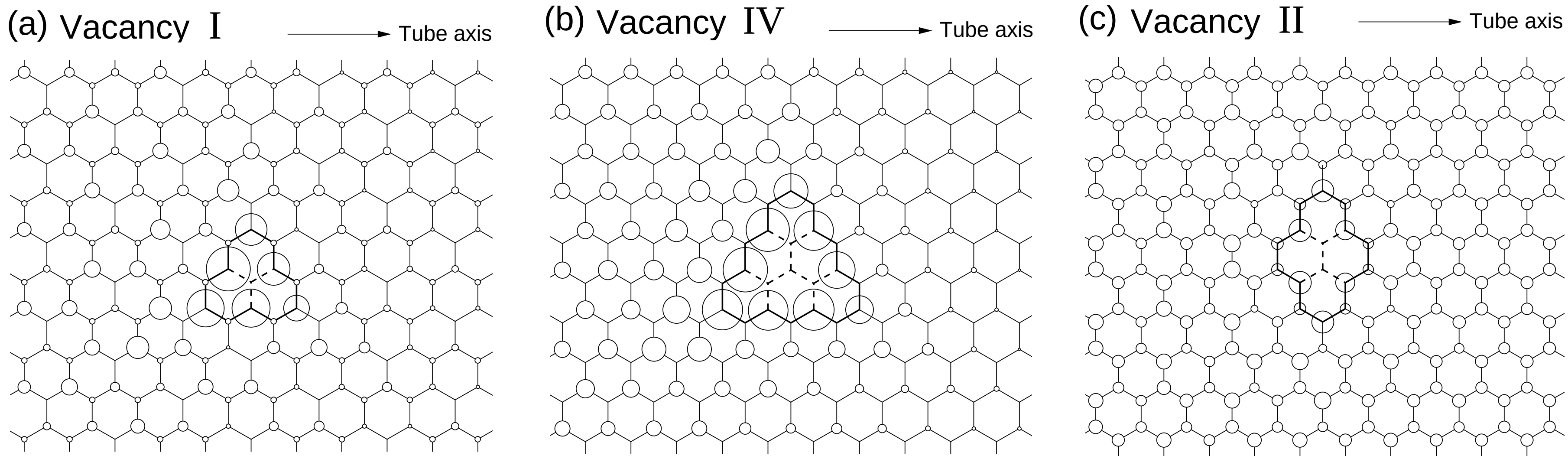
M. Igami, T. Nakanishi, and T. Ando, J. Phys. Soc. Jpn. **68**,716 (1999)



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



Wave Functions at $\varepsilon = 0$

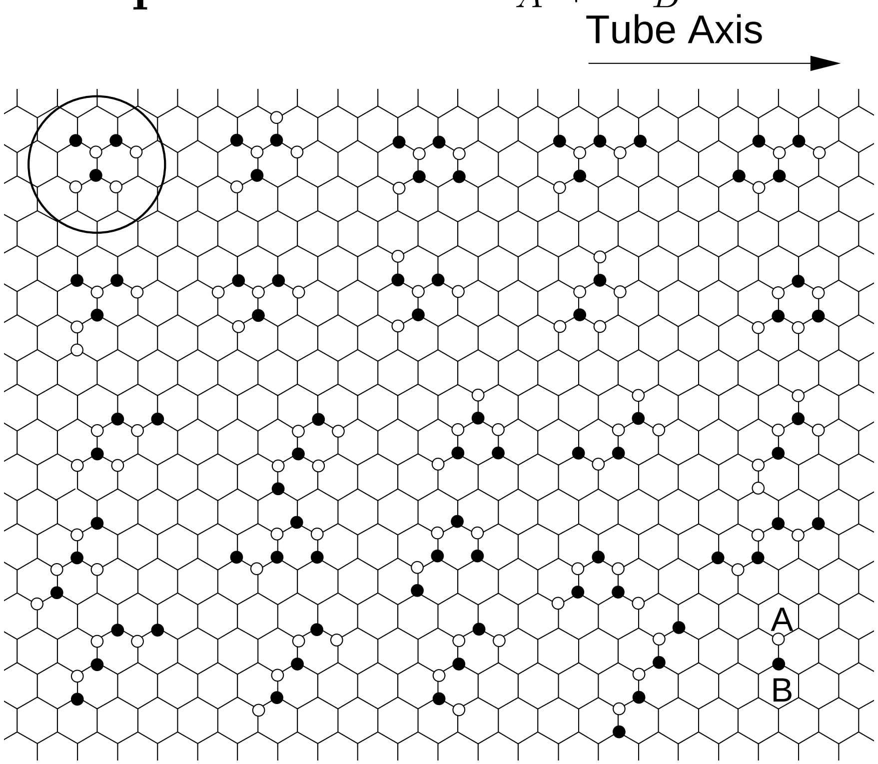


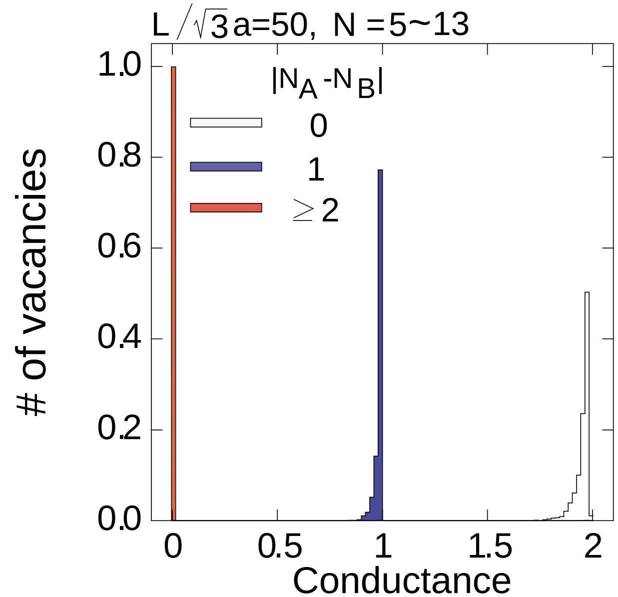
1. **Vacancy I: three sublattice Kekulé pattern Standing Wave (K and K' point)**
2. **Vacancy IV: Large amplitude at B sites no component on A sites (left-hand side)**
3. **Vacancy II: not disturbed by the vacancy**

Quantization Rule at $\varepsilon = 0$

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

Examples for $N = N_A + N_B = 7$





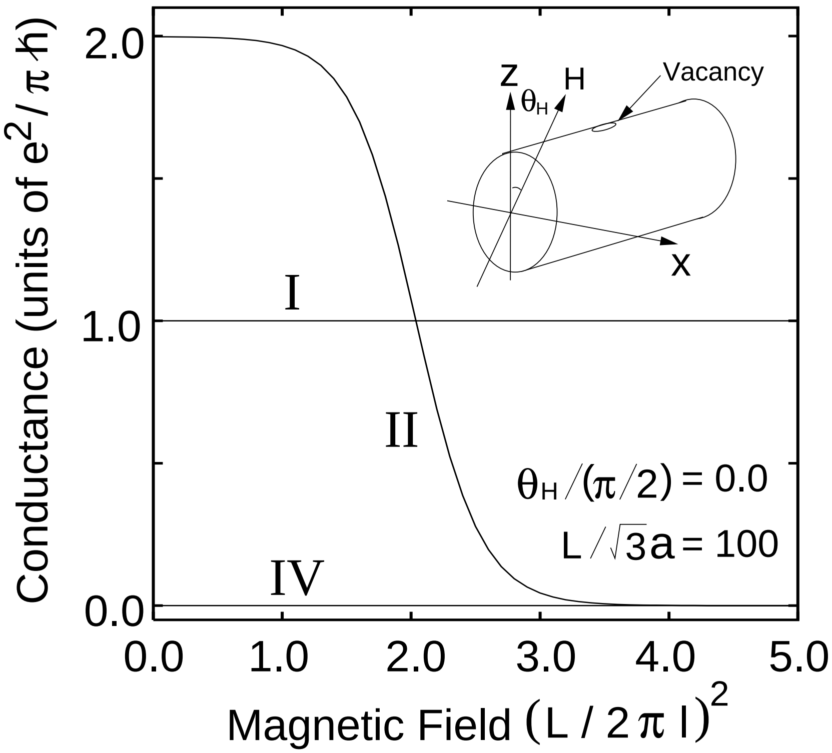
Quantization Rule at $\varepsilon = 0$

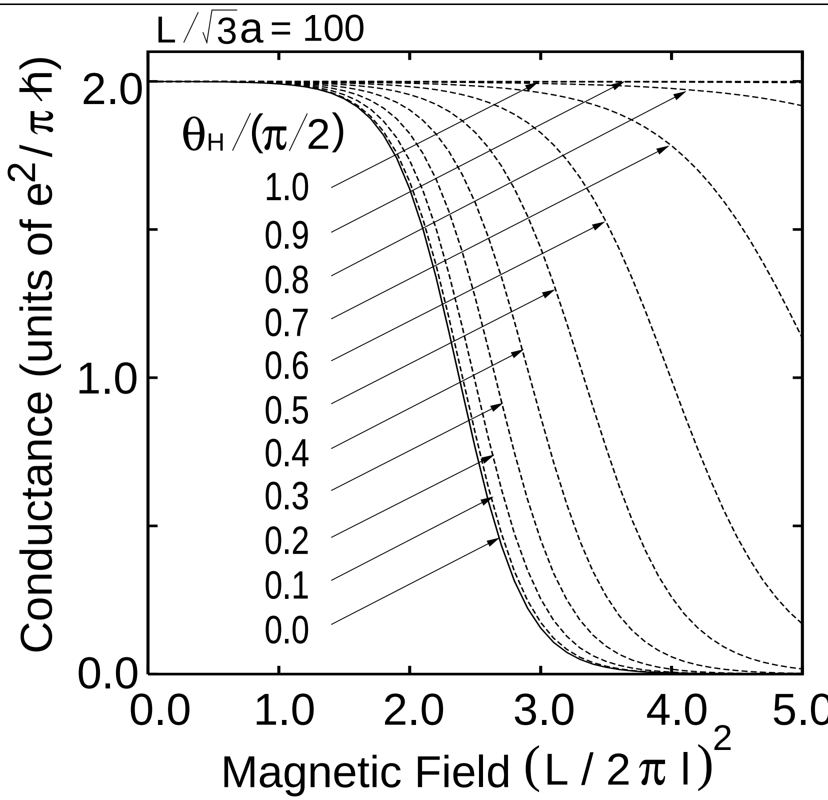
N_A, N_B: **number of removed A and B sublattice sites**

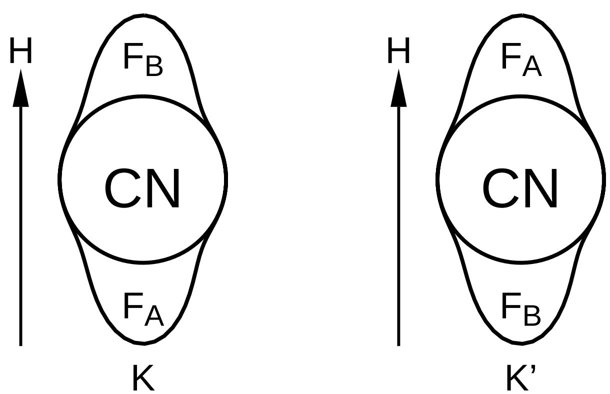
1.6×10^5 **different CN's with a vacancy**

$\|N_A - N_B\|$	**1**	**The Others (≥ 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,

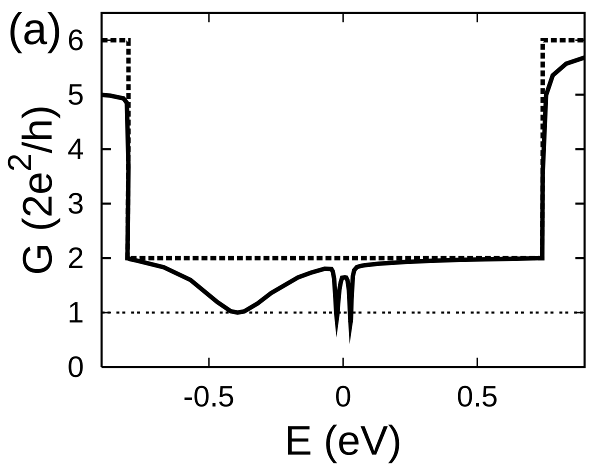
J. Phys. Soc. Jpn. **68**,716 (1999)

Defects in Carbon Nanotubes

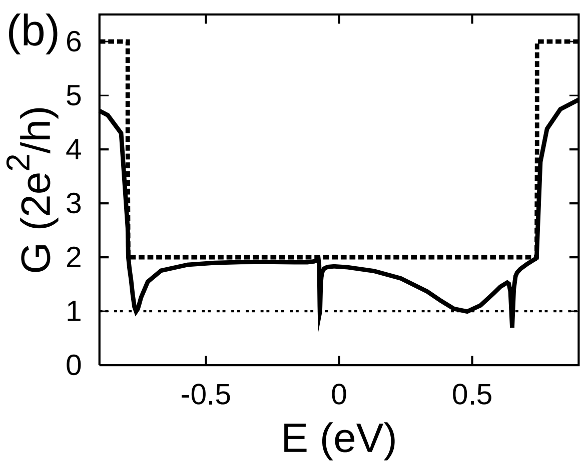
H. J. Choi, *et al.* PRL **84**, 2917 (2000)

ab initio study on transport in CN with B and N

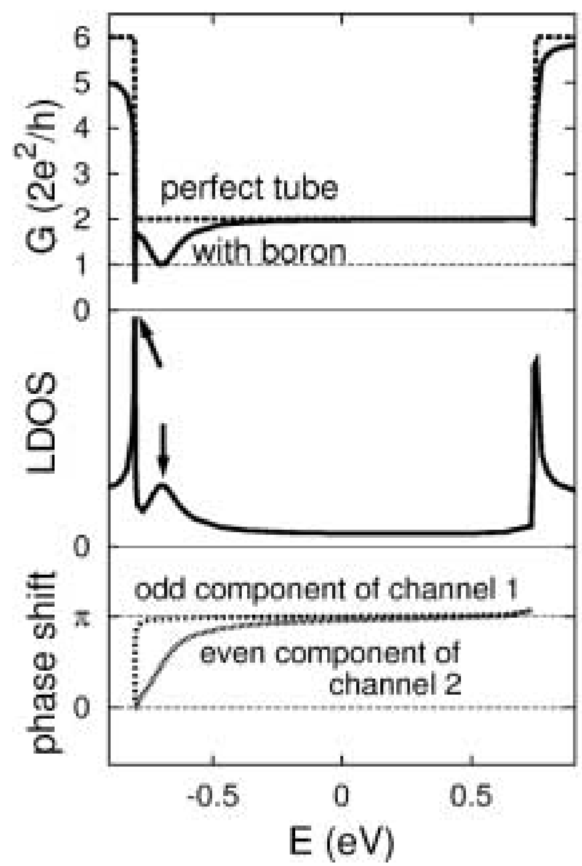
Point vacancy



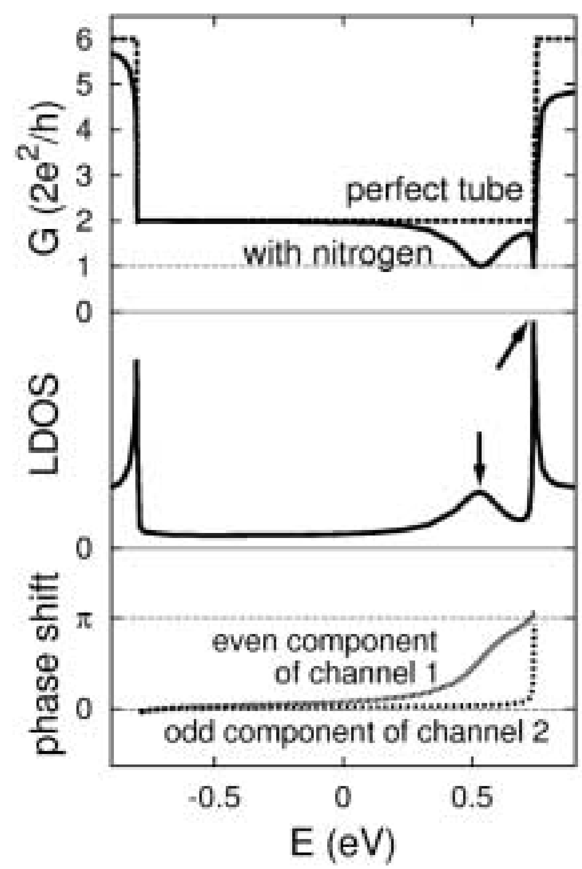
Double vacancy



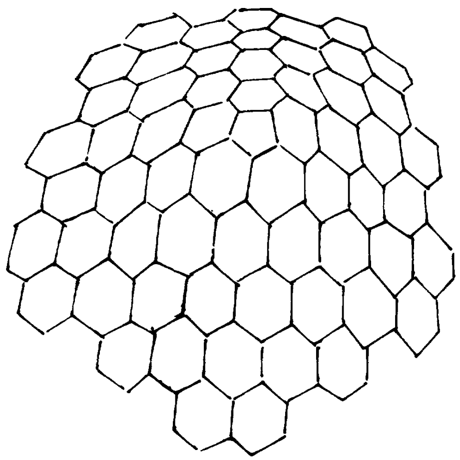
Boron: Acceptor

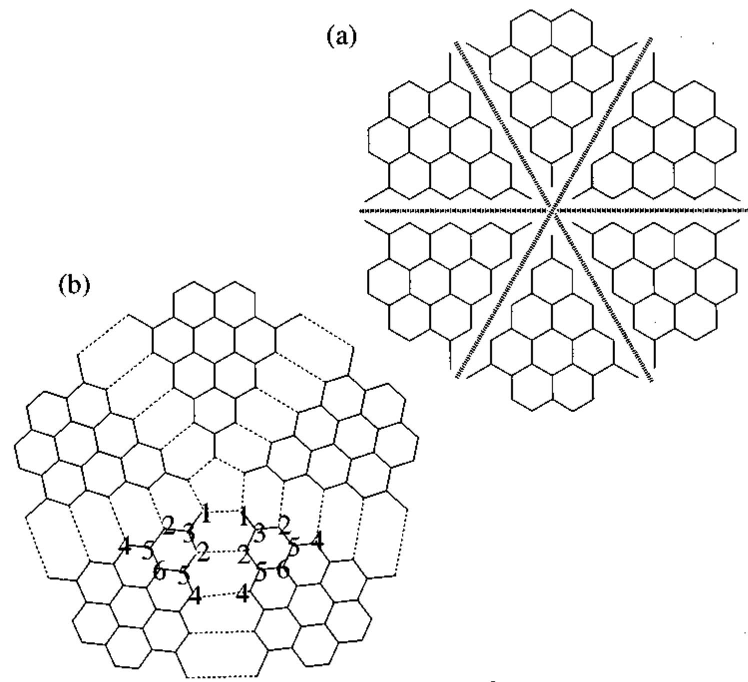


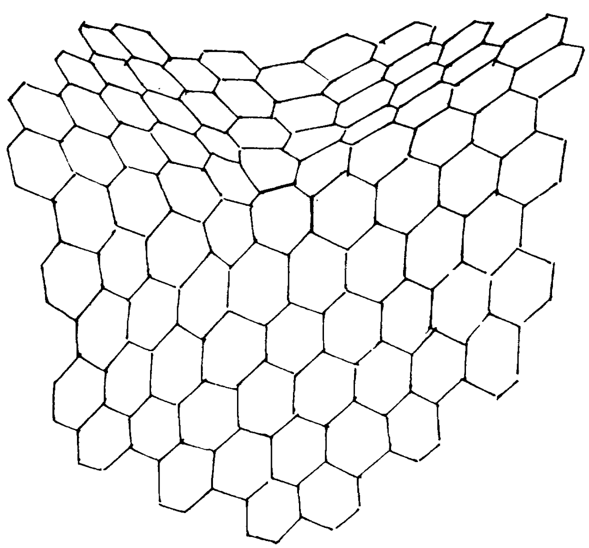
Nitrogen: Donor

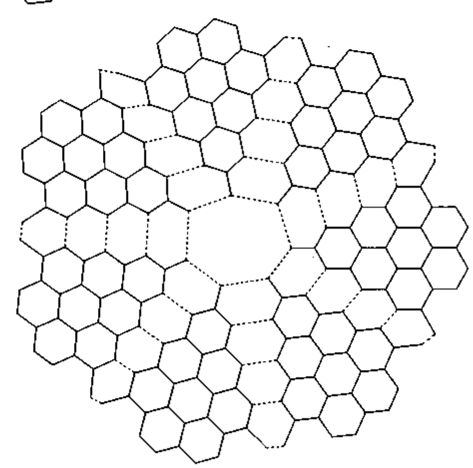


Topological Defects





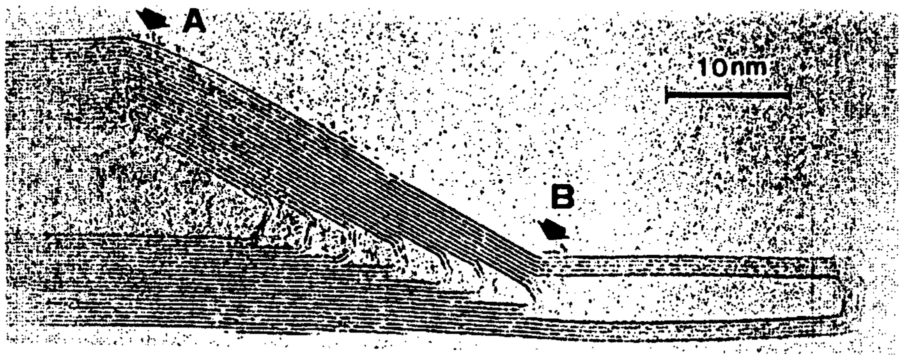


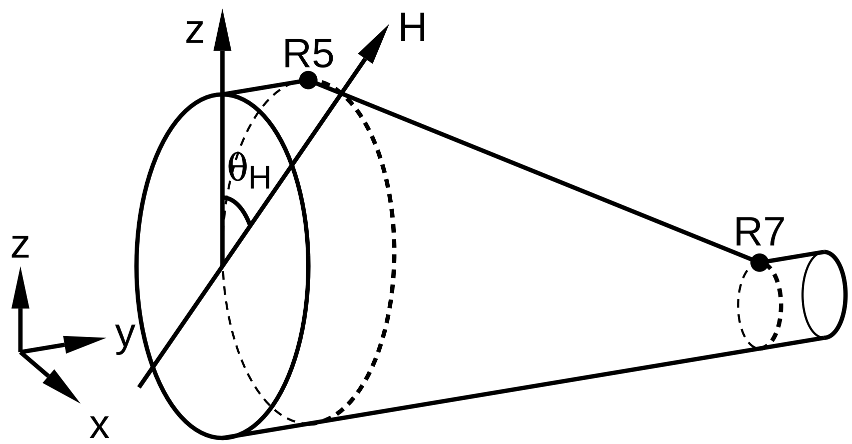


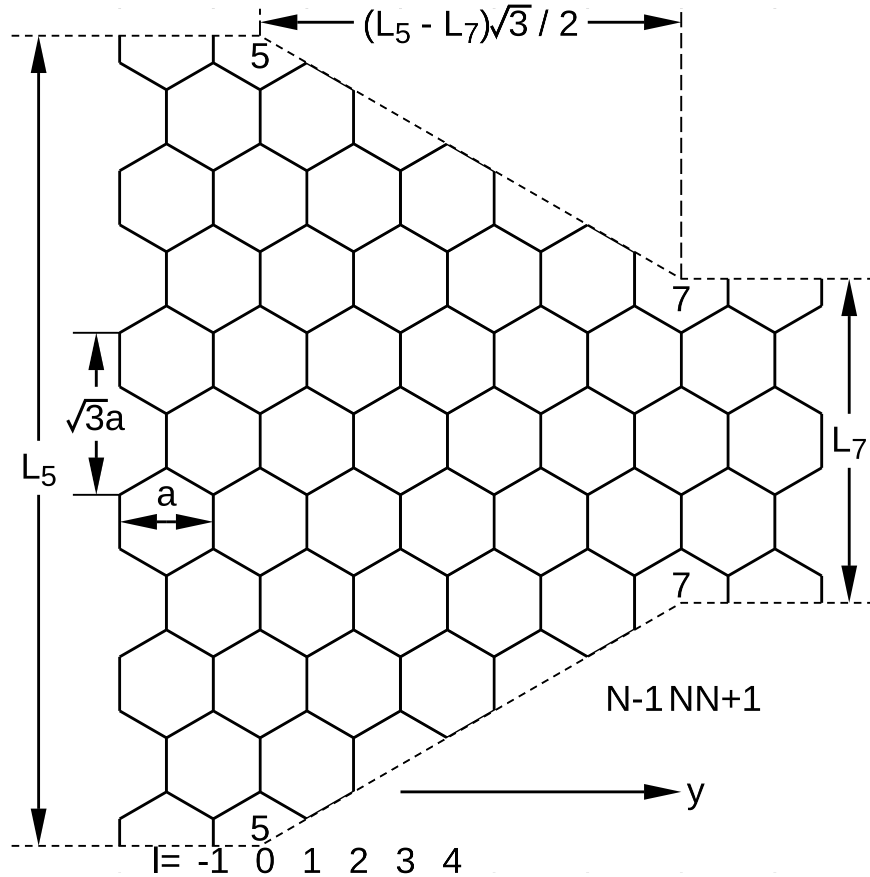
R. Tamura, *et al*. PRB **56** (1997) 1404; **49** (1994) 7697

Carbon Nanotube Junction

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





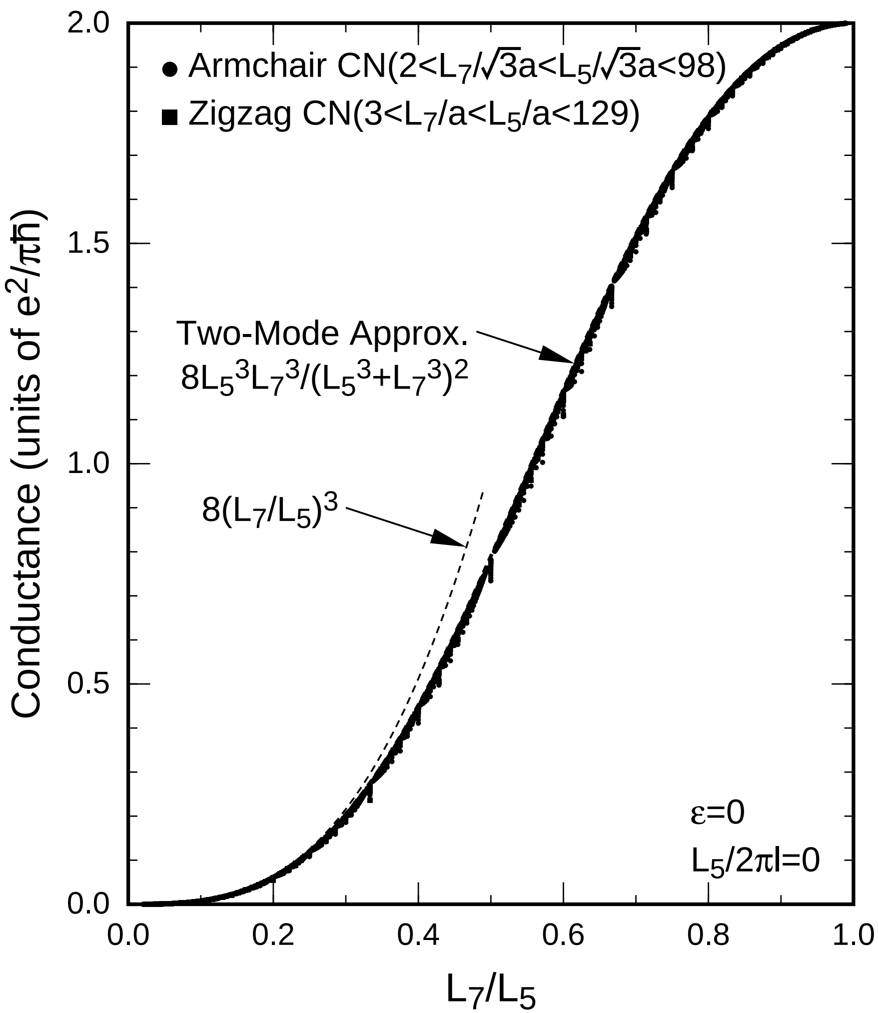


R5 (A): five-membered ring

R7 (B): seven-membered ring

Conductance of CN Junctions ($H = 0$)

R. Tamura and M. Tsukada, PR**B55**, 4991 (1997).



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

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

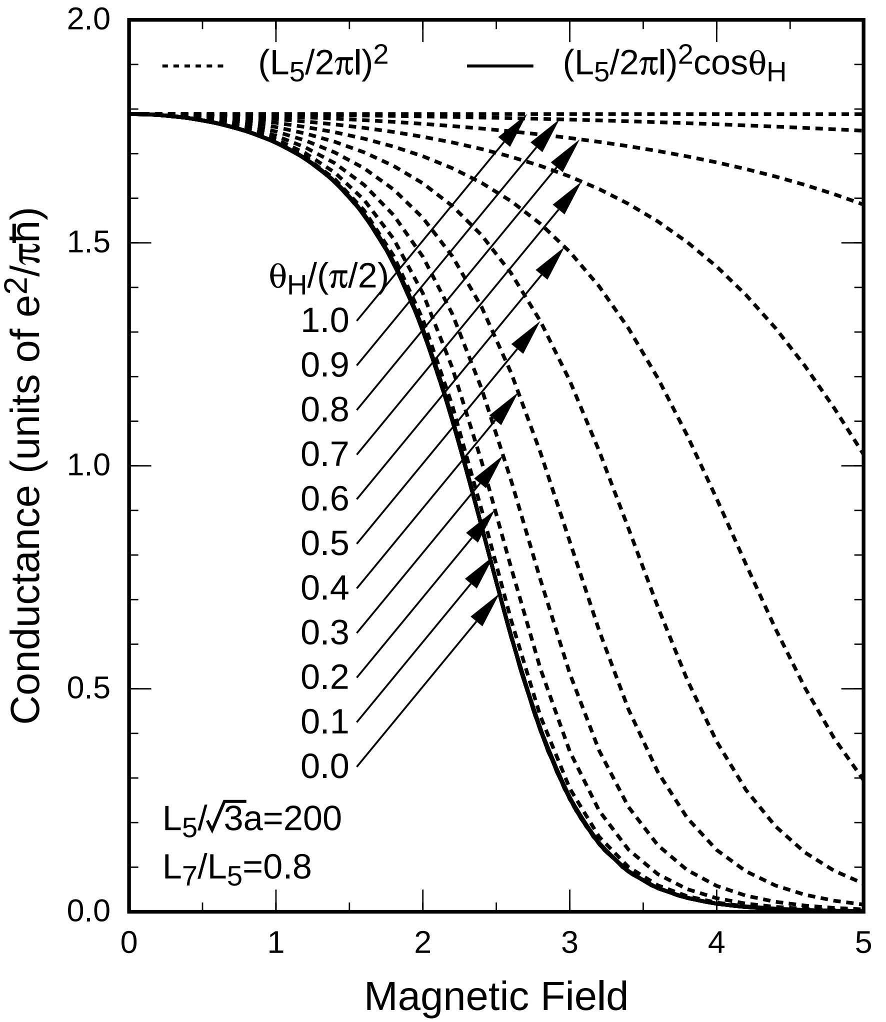
Effective-Mass Theory

Wave function decay linearly

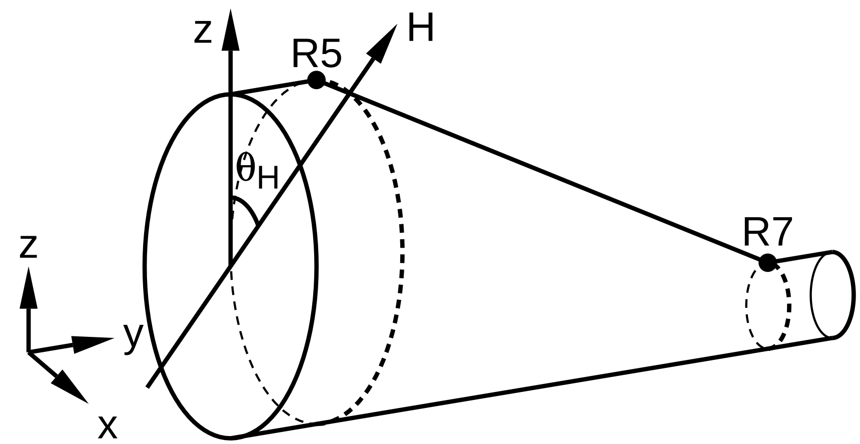
H. Matsumura and T. Ando, J. Phy. Soc. Jpn., **67**, 3542 (1998).

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. $H\cos\theta_H$

α

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 accepter
3. **Carbon Nanotube Junctions**