Graduiertenkolleg

Nichtlinearität und Nichtgleichgewicht in kondensierter Materie

15:00-, 18. Nov. 2004
Condensed matter theory seminar
Univ. Regensburg, Germany

# Transport through One-Dimensional Correlated Electrons with Electron-Phonon Interaction


Wataru Izumida

*Dept. of Phys., Tohoku Univ., Japan*

東北大学 TOHOKU UNIVERSITY

*Kavli Institute of Nanoscience, TU Delft, The Netherlands*


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TU Delft
Delft University of Technology
Faculty Of Applied Sciences

NanoScience


Collaboration: Milena Grifoni

*Dept. of Phys., Univ. of Regensburg, Germany*

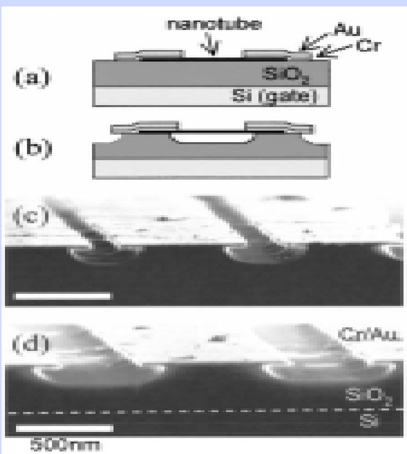


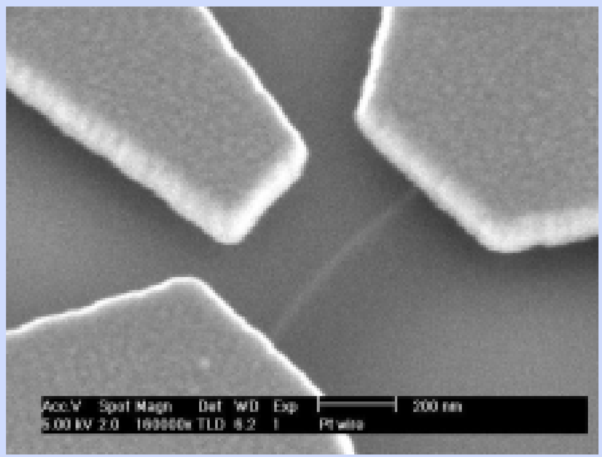
Thanks: Leonhard Mayrhofer (QTD, Univ. Regensburg), Graduiertenkolleg

# Motivated by,

## ***Free-standing Carbon Nanotube***

### Under-etching

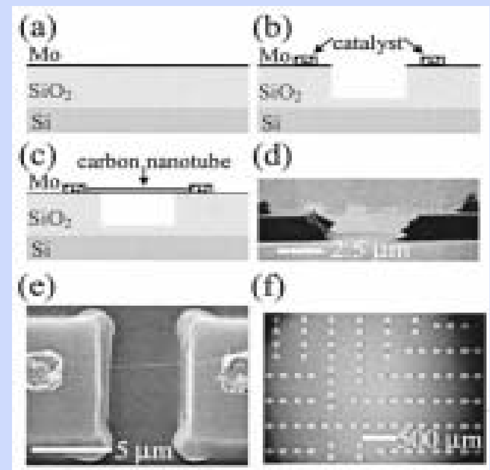



J. Nygard et al.:
Appl. Phys. Lett. 79, 4216 (2001)

S. Sapmaz et al. (TU Delft), unpublished.

### Growth “bridge” in CVD



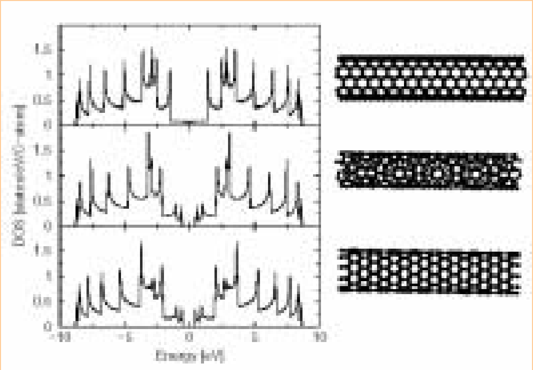

N. Franklin et al.:
Appl. Phys. Lett. 81,913(2002)

**What’s expected in FSNT?**

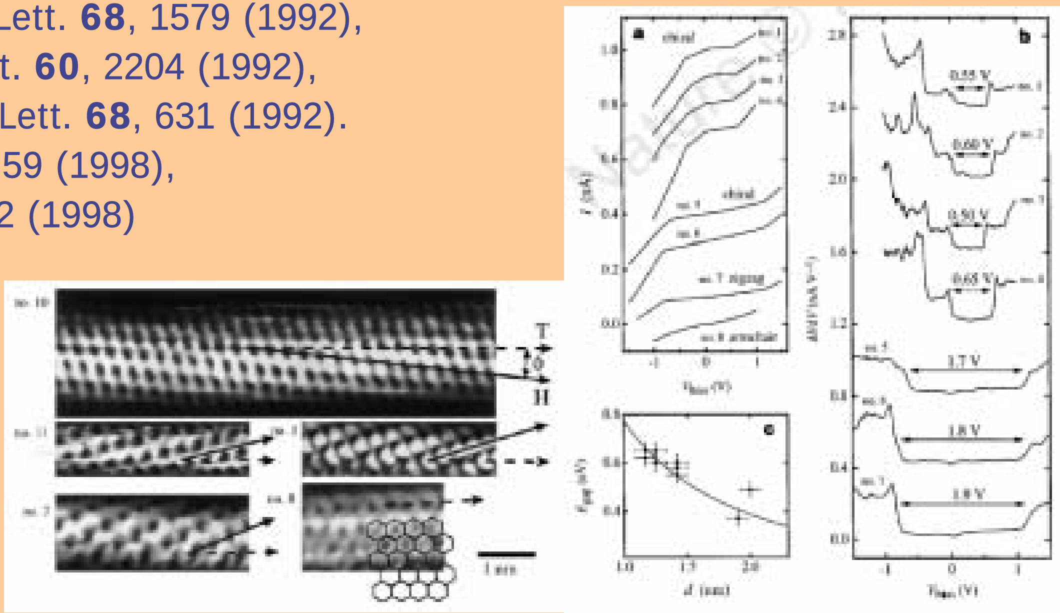
# Contents

# *Transport through Carbon Nanotubes*

- chirality: **metal** or **semiconductor**
  - Hamada et al., Phys. Rev. Lett. **68**, 1579 (1992),
    Saito et al., Appl. Phys. Lett. **60**, 2204 (1992),
    Mintmire et al., Phys. Rev. Lett. **68**, 631 (1992).
  - Wildoer et al. Nature **391**, 59 (1998),
    Odom et al. Nature **391**, 62 (1998)



Tight-binding calc.: by Saito et al.

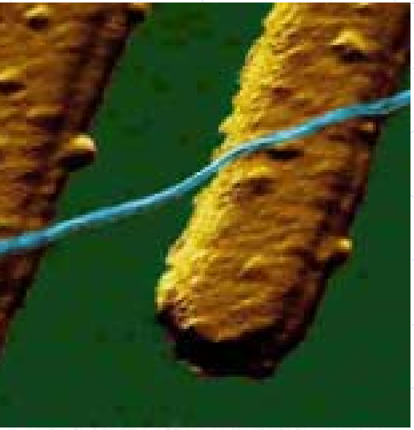


STM measurements: Wildoer et al. Nature 391, 59 (1998)

single-particle quantum mechanics

- **Electron correlation effect**

# Electron correlation in nanotube I.

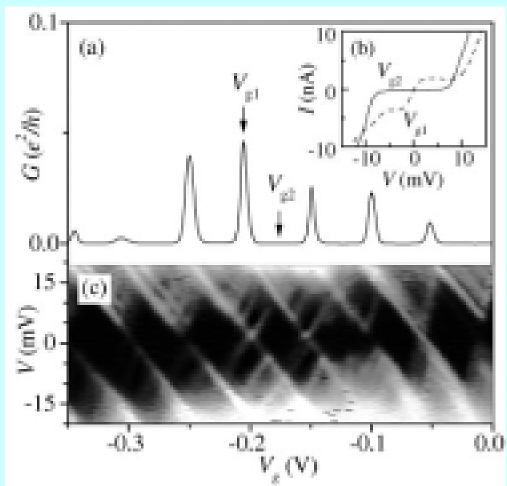


AFM image of an individual carbon nanotube between Pt electrodes spaced by 50 nm. Tans et al., Nature 386 (1997) 474.

Similer effect to quantum dot:

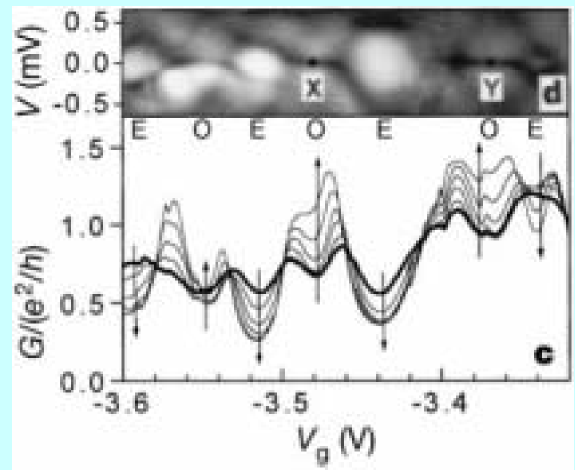
**Electron Correlation in 1-Dim "Quantum Dot"**

## Coulomb blockade




Nygard et al.:Appl. Phys. A 69, 297 (1999)

## Kondo effect




Nygard et al.: Nature 408, 342 (2000)

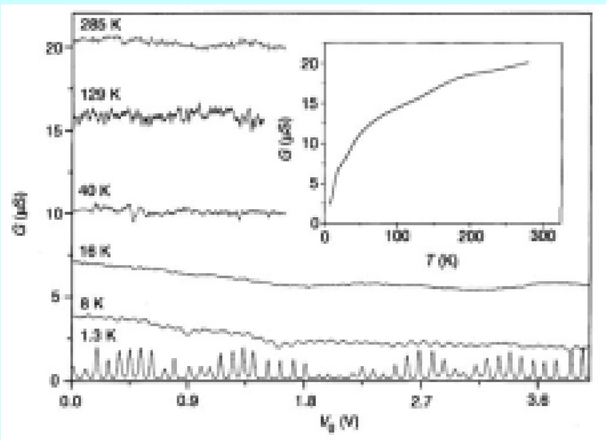
**$N_d$ changes one by one; reflecting strong U**

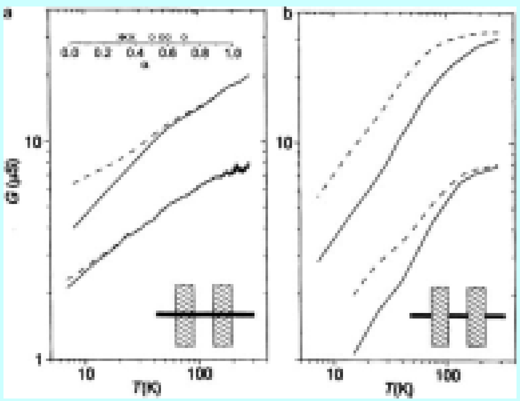
# Electron correlation in nanotube II.

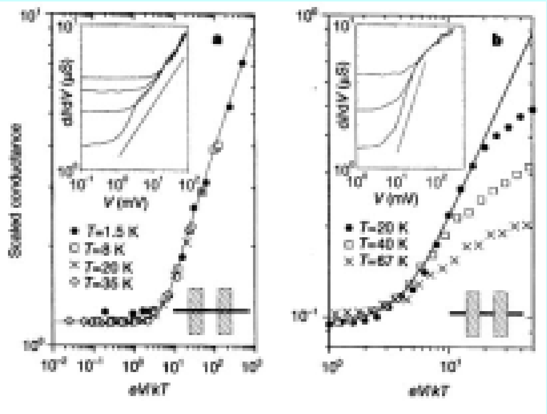
## Electron Correlation in "One-Dimension Conductor"

**Tomonaga-Luttinger liquid:**

**- power-law of G:** $G \sim \omega^{\alpha\_end}$, $G \sim \omega^{\alpha\_bulk}$



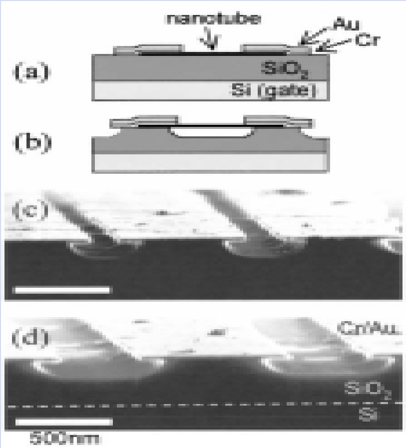

M. Bockrath et al.: Nature 397, 598 (1999)

Coulomb blockade, Kondo effect, TL Liquid

→Importance of **Electron Correlation** in CNT

# Free-standing Nanotubes

## Under-etching

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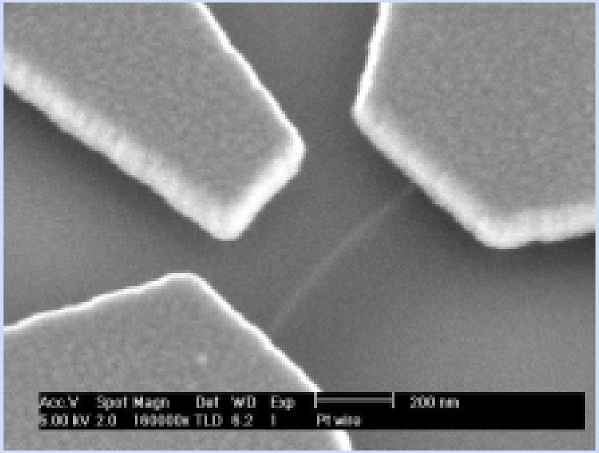


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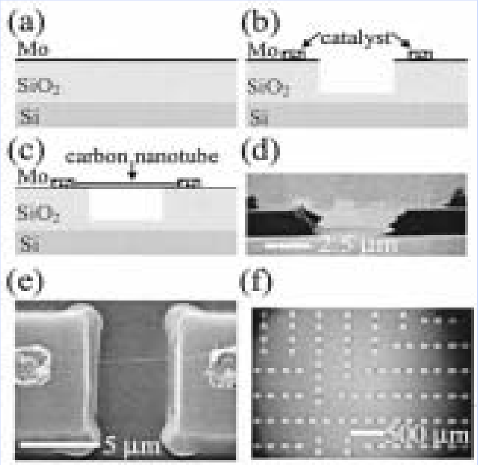
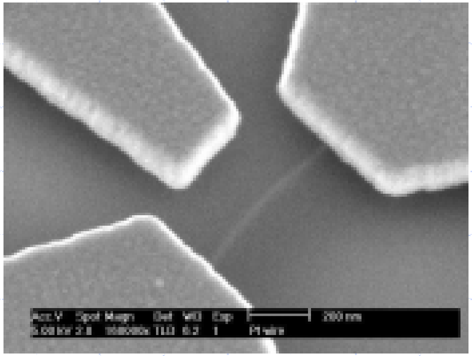



N. Franklin et al.:
Appl. Phys. Lett. 81,913(2002)

**What’s expected in FSNT?**

# Free-standing Carbon Nanotube

- Suppression of disorder: without substrate
- **"Beam"** fixed at its ends
  - Bending:
    - Change the capacitance
      - Sapmaz et al. PRB **67**, 235414 (2003)
  - **Vibration:**
    - induce phonon excitation in NT



Sapmaz et al. Unpublished.

— Purpose —

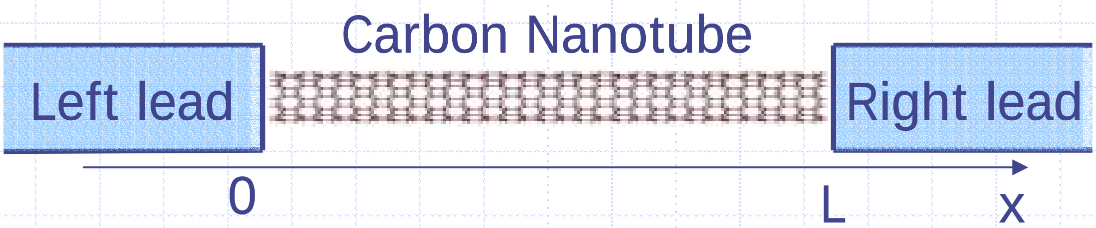
**How the mechanical motion affects the electrons?**

↓

*This talk: "1-dim. corr. electrons + el.-phonon coupling" in CNT*

# *Model of FSNT*

- Hamiltonian of the systems

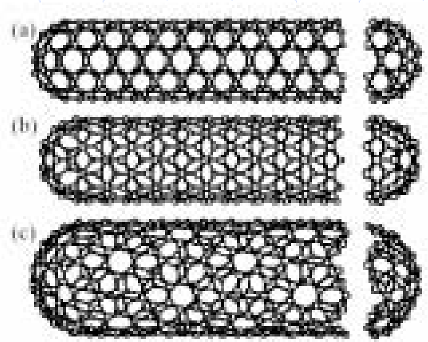



**- metallic Single-Walled NT**

**- Finite length, L, of CNT**

# Electronic structure of SWNT

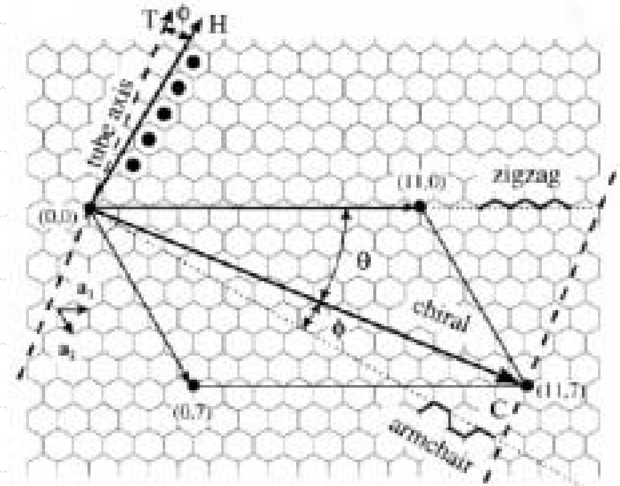
- Single-Walled Carbon Nanotube
  - -wrapped graphite sheet
  - -wrapping vector: $n\mathbf{a}_1 + m\mathbf{a}_2 := (n,m)$



**(5,5): armchair**

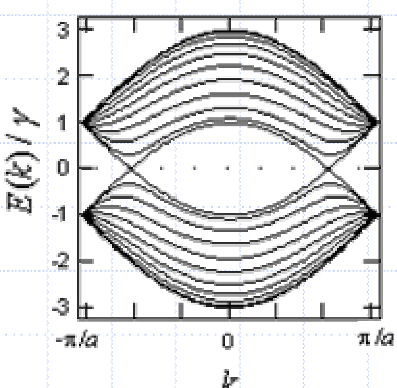
**(9,0): zigzag**

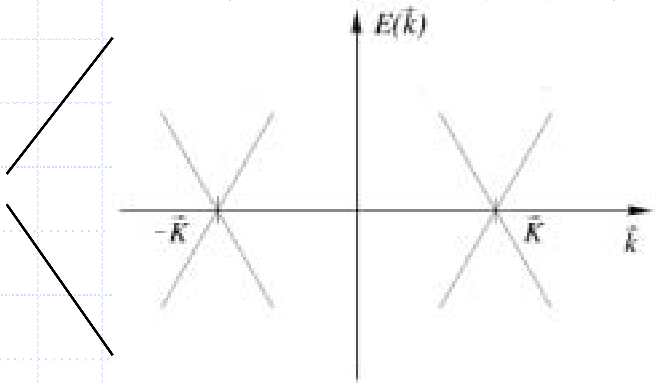
**(10,5): chiral**




$\mathbf{a}_1$, $\mathbf{a}_2$: graphite primitive lattice vectors

- n-m=3l: metal, 2 bands at $E_F$
  - -**1D conductor with 2 linear bands** in low energy



# TL model for electrons in CNT

- **1-dim. correlated electrons**: TL liquid
- **2 bands** in CNT → 4 sectors (total charge, total spin, relative charge, relative spin; j=ρ+, σ+, ρ−, σ−)
- **Long-range Coulomb interaction**:
  - only forward scattering: interaction parameters $g_{\rho+}<1$, $g_{\rho-}=g_{\sigma+}=g_{\sigma-}=1$
- **Finite length**:
  - open boundary condition
  - discreteness of the excitations
  - charging energy

## 1-dim. bosonized Hamiltonian:

Egger et al., PRL **79**, 5082 (1997), Eur. Phys. J. B **3**, 281 (1998)
Kane et al., PRL **79**, 5086 (1997).

$$H=\sum_j H_j$$

$$H_j=\frac{v_j}{2}dx\int_0^L\left[g_j\Pi_j^2(x)+\frac{1}{g_j}\left(\partial_x\phi_j(x)\right)^2\right]$$

$$=\sum_{n\geq 1}\Delta\varepsilon_j n\left(b_{jn}^{+}b_{jn}+\frac{1}{2}\right)+\frac{\Delta\varepsilon_j}{8g_j}N_j^2$$

$$g_{\rho+}=g=1/\sqrt{\left(1+\frac{U}{\pi\hbar v_F}\right)},\quad \left(U=8e^2\log\frac{R_s}{R}\right),\quad g_j=1\ \ (j=\rho-,\sigma+,\sigma-)$$

$$v_j=\frac{v_F}{g_j},\quad \Delta\varepsilon_0=\hbar v_F\frac{\pi}{L},\quad \Delta\varepsilon_j=\frac{\Delta\varepsilon_0}{g_j}$$

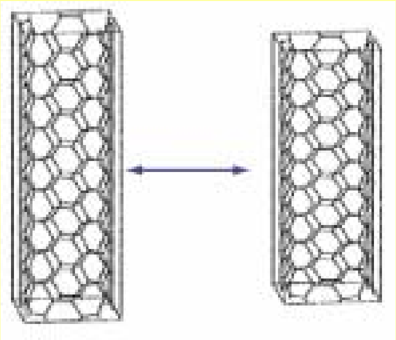
$$\phi(x)=\sqrt{\frac{2}{L}}\sum_{n\geq 1}\sin(k_n x)\phi_n,\quad \phi_n=\sqrt{\frac{\hbar g}{2k_n}}(b_n^{+}+b_n)\qquad k_n=\frac{n\pi}{L}$$

$$\Pi(x)=\sqrt{\frac{2}{L}}\sum_{n\geq 1}\sin(k_n x)\Pi_n,\quad \Pi_n=i\sqrt{\frac{\hbar k_n}{2g}}(b_n^{+}-b_n)$$

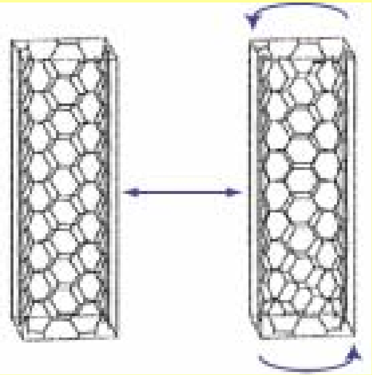
$N_j$: ground state occupation number in j-sector

# Phonons in CNT

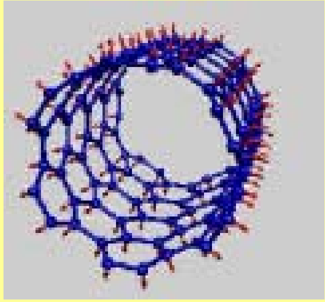
stretching mode



twisting mode



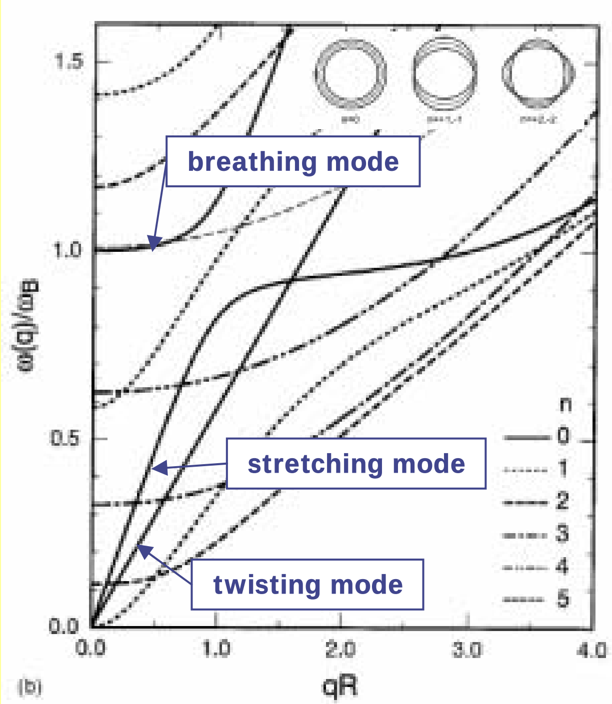
breathing mode



http://www-g.eng.cam.ac.uk/edm/research/ramanlab/raman_CNTs.html

- Phonon modes in CNT
  - **Stretching mode**:
    <->LA phonon in 1-dim.
  - Twisting mode:
    doesn't couple to electrons
  - Breathing mode:
    finite energy $\omega_B$ at k=0,
    negligible in low energy properties

phonon dispersion relation




Suzuura et al., PRB **65**, 235412 (2002)

# Phonon in CNT

- LA phonon in 1-dim. (<-> **stretching mode**)
- continuum model

## Phonon Hamiltonian: Longitudinal wave ($u_x \neq 0$)

$$H_{ph}^{lon} = \int_0^L dx \left[ \frac{1}{2\rho S} P_x^{\;2}(x) + \frac{ES}{2} \left( \partial_x u_x(x) \right)^2 \right]$$

$$= \sum_{n \geq 1} \Delta\varepsilon_a n \left( a_n^+ a_n + \frac{1}{2} \right)$$

ρ : Density of mass
E : Young's modulus
S: Cross-section

$$\Delta\varepsilon_a = \sqrt{\frac{E}{\rho}} \frac{\pi}{L}$$

$u_x$: displacement
P: conjugate momentum

$$u_x(x) = \sqrt{\frac{2}{L}} \sum_{n \geq 1} \sin(k_n x) u_{x,n}, \quad u_{x,n} = \sqrt{\frac{\hbar}{2\rho S \omega_n^{lon}}} (a_n^{\;+} + a_n)$$

$$\Pi_x(x) = \sqrt{\frac{2}{L}} \sum_{n \geq 1} \sin(k_n x) \Pi_{x,n}, \quad \Pi_{x,n} = i \sqrt{\frac{\hbar \rho S \omega_n^{lon}}{2}} (a_n^{\;+} - a_n)$$

# Electron-phonon interaction

## Deformation potential:

- $\propto \partial_x u_x(x)$
- interact with total charge density: **couple only to $H_{\rho+}$ term**

## Electron-phonon interaction:

$$H_{el-ph}^{lon} = c_{lon} \int dx\, \psi^+(x)\psi(x)\partial_x u_x(x)$$

$$= c_{lon} \int_0^L dx \left\{ \frac{1}{\sqrt{\pi\hbar}} \sqrt{\frac{2}{L}} \sum_{n\geq 1} k_n \cos(k_n x)\phi_{\rho+,n} + \rho_{q=0} \right\} \left\{ \sqrt{\frac{2}{L}} \sum_{n\geq 1} k_n \cos(k_n x) u_{x,n} \right\}$$

$$= \sum_{n\geq 1} \Delta I^{lon} n (b_{\rho+,n}^{\ +} + b_{\rho+,n})(a_n^{\ +} + a_n)$$

$$\Delta I^{lon} = c_{lon} \sqrt{\frac{\hbar g_{\rho+}}{4\pi S\sqrt{\rho E}} \frac{\pi}{L}}$$

$$\psi^+(x)\psi(x) = \frac{1}{\sqrt{\pi\hbar}} \partial_x \phi(x) + \rho_{q=0}$$

# Diagonalization of the Hamiltonian

## Total Hamiltonian: Bi-linear, diagonalized exactly

$$H_{\rho,total} = H_{\rho+} + H_{ph}^{lon} + H_{el-ph}^{lon}$$

$$= \sum_{n\geq 1} \Delta\varepsilon_{\rho+} n \left( b_{\rho+,n}^{+} b_{\rho+,n} + \frac{1}{2} \right) + \sum_{n\geq 1} \Delta\varepsilon_{a} n \left( a_n^{+} a_n + \frac{1}{2} \right) + \sum_{n\geq 1} \Delta I^{lon} n (b_{\rho+,n}{}^{+} + b_{\rho+,n})(a_n{}^{+} + a_n)$$

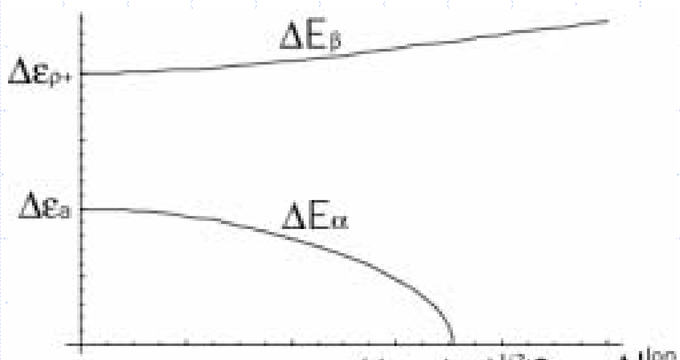
Bogoliubov transformation

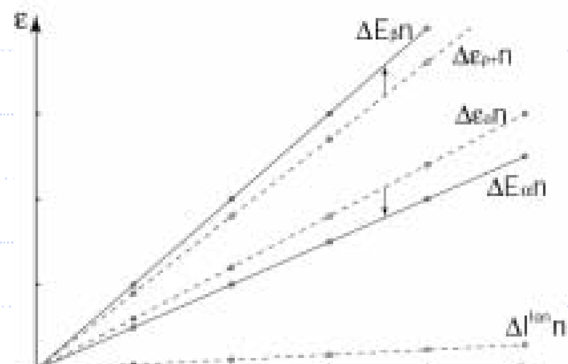
$$= \sum_{n\geq 1} \Delta E_{\beta} n \beta_n^{+} \beta_n + \sum_{n\geq 1} \Delta E_{\alpha} n \alpha_n^{+} \alpha_n + Const.$$

cf.
Engelsberg et al. PR **6A**, A1582 (1964),
Kleinert et al. Phys. Stat. Sol. (b) **199**, 435 (1997
etc…

where,

$$\Delta E_{\beta/\alpha} = \sqrt{\frac{(\Delta\varepsilon_{\rho+})^2 + (\Delta\varepsilon_b)^2}{2} \pm \sqrt{\left( \frac{(\Delta\varepsilon_{\rho+})^2 - (\Delta\varepsilon_b)^2}{2} \right)^2 + 4\Delta I^{lon} (\Delta\varepsilon_{\rho+})(\Delta\varepsilon_b)}}$$

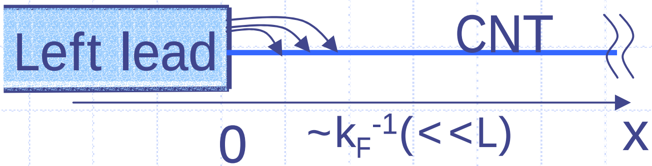


# *Current through CNT*

- Current formula
- Effect of deformation potential
  - infinite length: $L \to \infty$
  - finite length: $L \neq \infty$

# Current through CNT




**Current:**

- high enough barrier: lowest order of tunneling
- tunneling occurs only at the edge (~$k_F^{-1} \ll L$) region

**Differential conductance:**

$$\Rightarrow \frac{dI}{dV_{bias}} \propto -\frac{1}{\pi} \mathrm{Im}\, G_{1\mathrm{dim}}\left((x, x') = 0_+ ; V_{bias}\right) \equiv \rho_{end}\left(V_{bias}\right)$$

**DOS of end of NT**

# Infinite length limit (L→∞)

## Infinite length limit; high temperature (T≫ΔE~1/L)

spinless, single-band, for simplicity.

$$\rho_{end}(\omega) \propto |\omega|^{\frac{1}{g}-1} \rightarrow |\omega|^{\frac{1}{g'}-1}$$

$$(g')^{-1} = \left( \frac{\Delta E_\alpha}{\Delta \varepsilon_{\rho+}} \sin^2\varphi + \frac{\Delta E_\beta}{\Delta \varepsilon_{\rho+}} \cos^2\varphi \right) g^{-1} \approx \left(1 - a(\Delta I^{lon})^2\right) g^{-1}$$

$$\tan 2\varphi = -\frac{4\Delta I^{lon}\sqrt{\Delta\varepsilon_a \Delta\varepsilon_{\rho+}}}{\Delta\varepsilon_a{}^2 - \Delta\varepsilon_{\rho+}{}^2}$$

$\Delta I^{lon}$: electron-phonon interaction (>0),
a: constant (>0)

g': Renormalized interaction parameter (> g)
"contribution of **attractive** interaction"

For Carbon Nanotube:

$$\rho_{end}(\omega) \propto |\omega|^{\frac{1}{4}\left(\frac{1}{g_{\rho+}}+3\right)-1} \rightarrow |\omega|^{\frac{1}{4}\left(\frac{1}{g_{\rho+}'}+3\right)-1}$$

# Finite length CNT ($L \neq \infty$)

## Density of states at the end of CNT: $L \neq \infty$, $T \ll \Delta E$

$$\rho_{end}(\omega) = \sum_{p,q,r} C_{\alpha,p} C_{\beta,q} C_{\gamma,r} \delta\left(\omega - (E_c + p\Delta E_\alpha + q\Delta E_\beta + r\Delta\varepsilon_0)\right) + \sum_{p,q,r} C_{\alpha,p} C_{\beta,q} C_{\gamma,r} \delta\left(\omega + (E_c + p\Delta E_\alpha + q\Delta E_\beta + r\Delta\varepsilon_0)\right)$$

$C_p$: intensity of peaks

$E_c$: charging energy

$\Delta E_j$: discreteness

$$C_{\alpha,p} = C^{T=0}_{\alpha,p} + \alpha e^{-\Delta E_\alpha / k_B T}\left(C^{T=0}_{\alpha,p+1} + C^{T=0}_{\alpha,p-1} - 2C^{T=0}_{\alpha,p}\right)$$

$$C^{T=0}_{\alpha,p} = \frac{\Gamma(\alpha+p)}{p!\,\Gamma(\alpha)}\Theta(p)$$

$$\alpha = \frac{1}{4}\frac{1}{g}\frac{\Delta E_\alpha}{\Delta\varepsilon_b}\sin^2\varphi$$ :phonon

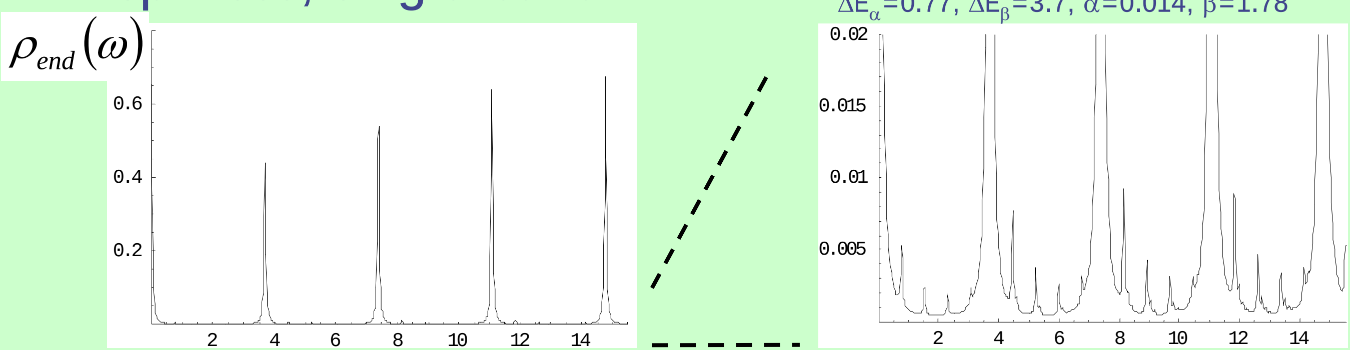
$$\beta = \frac{1}{4}\frac{1}{g}\frac{\Delta E_\beta}{\Delta\varepsilon_b}\cos^2\varphi$$ :charge

$$\gamma = \frac{3}{4}$$ : neutral modes

## spinless, single-band

$g=0.55$, $\Delta\varepsilon_a=1$, $\Delta\varepsilon_b=3.6$, $l=0.6$

$\Delta E_\alpha=0.77$, $\Delta E_\beta=3.7$, $\alpha=0.014$, $\beta=1.78$



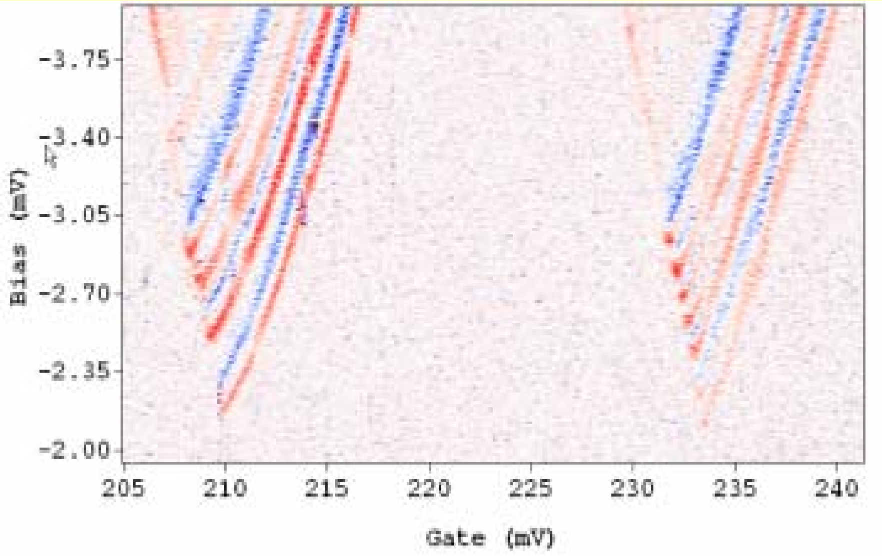

Discrete peaks

- discrete energies of charge density, neutral modes: $\Delta E_\beta$, $\Delta\varepsilon_0$
- n-phonons assisted tunneling: $\Delta E_\alpha$

Peak height: power law ($C_p \sim p^{\alpha-1}$)

# Compare with experiment

P. Jarillo-Herrero *et al* (TU Delft), unpublished.




- measure for L=1200nm metallic FS-SWNT, @T=300mK
- excitation peaks outside of Coulomb diamonds:
  - almost **same period**: $\Delta E_{exp}$~0.1 to 0.2meV

Estimated values; (for L=1μm)
$g_{\rho+}$~0.25~0.3, $\Delta\varepsilon_0=\hbar v_F\pi/L$**=0.7meV**, $\Delta\varepsilon_a$=0.06meV, $\Delta I^{lon}$=0.01meV
**→$\Delta E_\alpha$=0.06meV**, **$\Delta E_\beta$=2.8meV**

$\Delta E_{exp}$~$2\Delta E_\alpha$, $0.15\Delta\varepsilon_0$, $0.1\Delta E_\beta$: come from phonon?

# Summary & Future

- phonon effect in CNT
  - changing of power
  - phonon excitation peaks
  - compare with exp. (phonon peaks?)
- Other interests
  - gate voltage effect
    - Coulomb blockade
    - Int. between el. and TA phonon