Are Double Wall Nanotubes Luttinger Liquids?

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Electronic structure of graphene sheets





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$$H_0 = t_0 \sum_{\mathbf{k}} \gamma_{\mathbf{k}} c_{A\mathbf{k}}^{\dagger} c_{B\mathbf{k}} + \text{H.c.}, \qquad \gamma_{\mathbf{k}} = \sum_{j=1}^{k} e^{i\mathbf{k} \cdot \mathbf{d}_j}$$

Low energy theory

Expand around the Fermi point — $\mathbf{k} = \alpha \mathbf{K}_0 + \mathbf{q}, \quad \alpha = \pm$,

$$\gamma_{\mathbf{k}} = \sum_{j=1}^{3} e^{i\mathbf{k}\cdot\mathbf{d}_{j}} = \sum_{j=1}^{3} e^{i(\alpha\mathbf{K}_{0}+\mathbf{q})\cdot\mathbf{d}_{j}} \approx -\frac{3a_{0}}{2}(\alpha q_{x} - iq_{y})$$

The Hamiltonian becomes

$$H_0 = v\psi^{\dagger}_{\alpha\mathbf{k}} \left(\alpha q_x \sigma_x + q_y \sigma_y\right) \psi_{\alpha\mathbf{k}}$$

with

$$v = 3t_0 a_0/2,$$
 $\psi^{\dagger}_{\alpha \mathbf{k}} = (c^{\dagger}_{A\mathbf{k}}, c^{\dagger}_{B\mathbf{k}}),$ $q_y = \mu G_1$
 σ_x, σ_y Pauli Matrices

Structure of nanotubes (n,m) l





 $_1 + m\mathbf{a}_2$ Chiral (wrapping) vector for a tube (n,m)

Structure of nanotubes (n,m) II

• Unit lattice vectors $(a_0 = 1.42 \text{ Å})$

$$\mathbf{a}_1 = \sqrt{3}a_0(1/2, \sqrt{3}/2), \quad \mathbf{a}_2 = \sqrt{3}a_0(-1/2, \sqrt{3}/2)$$

• Chiral (wrapping) vector

$$\mathbf{h} = n\mathbf{a}_1 + m\mathbf{a}_2, \quad |\mathbf{h}| = \sqrt{3}a_0\mathcal{L}, \qquad \mathcal{L} = \sqrt{n^2 + m^2 + nm}$$

• The unit vector **T** along the tube axis

$$\mathbf{T} = \left((2n+m)\mathbf{a}_1 - (2m+n)\mathbf{a}_2 \right)/d_R, \qquad T = 3a_0\mathcal{L}/d_R$$

 d_R is the greatest common divisor of (2n+m) and (2m+n).

 $T = \sqrt{3}a_0$, armchair (m, n), $T = 3a_0$ zigzag (0, m)

Structure of nanotubes (n,m) III

• Number of hexagons in the nanotube unit cell

$$N = \frac{2(n^2 + m^2 + nm)}{d_R} = \frac{2\mathcal{L}^2}{d_R}$$

N=2m armchair (m,m), N=2m zigzag (0,m)

• Discrete unit wave vector along h:

$$\mathbf{G}_1 = \frac{(2n+m)\mathbf{b}_1 + (2m+n)\mathbf{b}_2}{Nd_R}, \qquad |\mathbf{G}_1| = \frac{2\pi}{h}$$

• Unit reciprocal lattice vector along T

$$\mathbf{G}_2 = \frac{(m\mathbf{b}_1 - n\mathbf{b}_2)}{N}, \qquad |\mathbf{G}_2| = \frac{2\pi}{T}$$

Structure of double wall nanotubes (DWNT)



(9,0)@(18,0) (up) and (9,0)@(10,10) (down)

*S. Roche et al., Phys. Lett. A 285, 94 (2001)

Electronic structure of single wall nanotube I

 $E_{\mu}(k) = E_{2D}(\mathbf{k})$ $\mathbf{k} = k\mathbf{G}_2/G_2 + \mu\mathbf{G}_1$ $\begin{cases} -\pi/T < k < \pi/T, \\ \mu = 1, 2, \dots, N \end{cases}$

N Number of subbands



 $\overline{(5,5)}$ nanotube

Electronic structure of single wall nanotube II

Condition for metallic tubes

$$\begin{aligned} \mathbf{G}_1 \cdot \mathbf{K}_0 / G_1 &= \mathsf{Integer} \\ \frac{\mathbf{G}_1 \cdot \mathbf{K}_0}{G_1} &= \frac{n - m}{3}, \\ \frac{\mathbf{G}_1 \cdot \mathbf{K}_1}{G_1} &= \frac{2m + n}{3}, \\ \frac{\mathbf{G}_1 \cdot \mathbf{K}_{-1}}{G_1} &= -\frac{2n + m}{3}, \end{aligned}$$

Armchair nanotubes (m, m) are always metallic! Coulomb interaction, electronic structure?



Why is 1D system special

- Fermi liquid
 - ★ Quasi particles
 - ★ Fermi surface



Luttinger liquid

- ★ No quasi particles
- ⋆ No Fermi surface
- ★ Tomonaga-Luttinger model



Tomonaga-Luttinger(TL) model

• It only describes low energy excitation near the Fermi energy E_F ,

$$E(k) \approx E_F + \frac{\hbar^2 k_F}{m} (k - k_F).$$

• The dispersion relation becomes linearized

$$E(k) = \hbar v_F(k - k_F), \qquad v_F = \hbar \frac{k_F}{m}$$

• Right- and left-movers

$$c_k = c_{+,k}\Theta(k) + c_{-,k}\Theta(-k)$$

• It is exactly solvable by bosonization technique!

Single wall nanotubes as Luttinger liquids I



$$\Psi_{\sigma}(x,y) = \sum_{p\alpha} \phi_{p\alpha}(x,y)\psi_{p\alpha\sigma}(x),$$

$$\psi_{r\alpha\sigma} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \psi_{p\alpha\sigma} \Leftrightarrow \psi_{p\alpha\sigma} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \psi_{r\alpha\sigma}.$$
$$H = -\hbar v \sum_{p\alpha\sigma} p \int dx \, \psi_{p\alpha\sigma}^{\dagger} \partial_x \psi_{-p\alpha\sigma} \quad \Rightarrow \quad H = -i\hbar v \sum_{r\alpha\sigma} r \int dx \, \psi_{r\alpha\sigma}^{\dagger} \partial_x \psi_{r\alpha\sigma}.$$

Single wall nanotubes as Luttinger liquids II

The Coulomb interaction



$$H_{\alpha FS}^{(0)} = \frac{1}{2} \int dx dx' \ \rho(x) V_0(x - x') \rho(x') \qquad \text{Forward scattering}$$

*R. Egger and A. O. Gogolin, Eur. Phys. J. B 3, 281 (1998)

Single wall nanotubes as Luttinger liquids III

The density operators

$$\rho(x) = \sum_{r\alpha\sigma} \psi^{\dagger}_{r\alpha\sigma}(x)\psi_{r\alpha\sigma}(x) = \sum_{r\alpha\sigma} \rho_{r\alpha\sigma}(x)$$

The Fermi field operator

$$\psi_{r\alpha\sigma}(x) = \frac{\eta_{r\alpha\sigma}}{\sqrt{2\pi a}} \exp(i\alpha k_F x + irq_F x + i\varphi_{r\alpha\sigma}(x))$$

with $\eta_{r\alpha\sigma}$ — Klein factor, a — cutoff, and

$$\varphi_{r\alpha\sigma} = \frac{\sqrt{\pi}}{2} (r\phi_{c+} + r\alpha\phi_{c-} + r\sigma\phi_{s+} + r\alpha\sigma\phi_{s-} + \Theta_{c+} + \alpha\Theta_{c-} + \sigma\Theta_{s+} + \alpha\sigma\Theta_{s-})$$

Hamiltonian with interactions can be easily diagonalized by these Bosonic operators!

Single wall nanotubes as Luttinger liquids IV

New boson operators

$$\begin{split} \phi_{c+} &= \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} r\varphi_{r\alpha\sigma}, & \Theta_{c+} &= \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} \varphi_{r\alpha\sigma}, & \text{total charge} \\ \phi_{c-} &= \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} r\alpha\varphi_{r\alpha\sigma}, & \Theta_{c-} &= \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} \alpha\varphi_{r\alpha\sigma}, & \text{relative charge} \\ \phi_{s+} &= \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} r\sigma\varphi_{r\alpha\sigma}, & \Theta_{s+} &= \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} \sigma\varphi_{r\alpha\sigma}, & \text{total spin} \\ \phi_{s-} &= \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} r\alpha\sigma\varphi_{r\alpha\sigma}, & \Theta_{s-} &= \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} \alpha\sigma\varphi_{r\alpha\sigma}, & \text{relative spin} \end{split}$$

The commutators of them are

$$[\phi_{j\delta}(x), \Theta_{j'\delta'}(x')] = i\frac{\pi}{2}\delta(x-x')\operatorname{sgn}(x-x')\delta_{j\delta,j'\delta'}.$$

Single wall nanotubes as Luttinger liquids V

Kinetic Hamiltonian

$$H_0 = \sum_{j\delta} \frac{\hbar v_{j\delta}^0}{2} \int dx \left(K_{j\delta}^0 \left(\partial_x \Theta_{j\delta}(x) \right)^2 + \frac{1}{K_{j\delta}^0} \left(\partial_x \phi_{j\delta}(x) \right)^2 \right),$$

with $j = c, s, \delta = \pm, v_{j\delta}^0 = v = v_F$ and $K_{j\delta}^0 = 1$. Interaction Hamiltonian (only affect c + mode)

$$H_{\alpha FS}^{(0)} = \frac{2}{\pi} \int dx dx' \,\rho(x) V(x - x') \rho(x')$$
$$= \int \frac{dk}{2\pi} \frac{2k^2 V(k)}{\pi} e^{-ikx} \phi_{c+}(k) \phi_{c+}(-k).$$

Forward scattering

with $\rho(x) = \frac{2}{\sqrt{\pi}} \partial_x \phi_{c+.}$

Single wall nanotubes as Luttinger liquid VI

The total Hamiltonian

$$H_0 + H_{\alpha FS}^{(0)} = \sum_{j\delta} \int \frac{dk}{2\pi} \frac{\hbar v_{j\delta}}{2} \left(K_{j\delta} \Pi_{j\delta}(k) \Pi_{j\delta}(-k) + \frac{k^2}{K_{j\delta}} \phi_{j\delta}(k) \phi_{j\delta}(-k) \right),$$

with

$$v_{c+}(k) = v\sqrt{1 + \frac{4V(k)}{\pi v}}, \quad K_{c+} = \sqrt{\frac{1}{1 + 4V(k)/\pi v}},$$
$$v_{j\delta} = v, \qquad K_{j\delta} = 1 \quad \text{others}$$

The Hamiltonian can be diagonalized by Bogliugov transformation. The energy spectrum of each mode is

$$E_{j\delta}(k) = \hbar v_{j\delta}k$$

Interlayer coupling in DWNTs I

Tunneling Hamiltonian





 $t_{ai,bj}e^{i(\mathbf{k}_b\cdot\mathbf{r}_b-\mathbf{k}_a\cdot\mathbf{r}_a)}c^{\dagger}_{i\eta_a\mathbf{k}_a}c_{j\eta_b\mathbf{k}_b} + \text{H.c.},$

a, b — indices for atoms, i, j — indices for two walls, N_a, N_b — numbers of unit cell.

The position of a lattice site $\mathbf{r}_i = \mathbf{R} + \boldsymbol{\rho} + \eta \boldsymbol{\tau}$, where R — lattice vector.

$$\frac{1}{A_{\text{cell}}} \sum_{\mathbf{G}} e^{-i\mathbf{G}\cdot\mathbf{R}} = \delta(R) \quad \Rightarrow \quad \sum_{\mathbf{R}} = \int d\mathbf{r}\delta(\mathbf{R}) = \frac{1}{A_{\text{cell}}} \sum_{\mathbf{G}} \int d\mathbf{r} e^{-i\mathbf{G}\cdot\mathbf{R}}$$

G — reciprocal lattice vector, A_{cell} — area of an unit cell

Interlayer coupling in DWNTs II

Expand around Fermi points $\mathbf{k} = \alpha \mathbf{K_0} + \mathbf{q}$, the Hamiltonian becomes

$$H_t = \sum_{\alpha_a \alpha_b} \sum_{\eta_a \eta_b} \sum_{\mathbf{q}_a} \psi^{\dagger}_{\alpha_a \mathbf{q}_a} \mathbf{q}_b T(\alpha_a \eta_a \mathbf{q}_a, \alpha_b \eta_b \mathbf{q}_b) \psi_{\alpha_b \mathbf{q}_b}$$

with $\psi^{\dagger}_{i\alpha \mathbf{q}} = (c^{\dagger}_{iA\mathbf{k}}, c^{\dagger}_{iB\mathbf{k}})$, $\eta = \pm$ — indices for sublattices.

$$T(\alpha_a \eta_a \mathbf{q}_a, \alpha_b \eta_b \mathbf{q}_b) = \sum_{\mathbf{K}_a \mathbf{K}_b} e^{i\mathbf{K}_a \cdot (\boldsymbol{\rho}_a + \eta_a \boldsymbol{\tau}_a) - i\mathbf{K}_b \cdot (\boldsymbol{\rho}_b + \eta_b \boldsymbol{\tau}_b)} t_{\mathbf{q}_a + \mathbf{K}_a, \mathbf{q}_b + \mathbf{K}_b}$$

and

$$t_{\mathbf{k}_{a},\mathbf{k}_{b}} = \frac{1}{A_{\text{cell}}^{2}\sqrt{N_{a}N_{b}}} \int d\mathbf{r}_{a} d\mathbf{r}_{b} e^{i(\mathbf{k}_{b}\cdot\mathbf{r}_{b}-\mathbf{k}_{a}\cdot\mathbf{r}_{a})} t_{ai,bj}$$

*A. A. Maarouf et al., PRB **61**, 11156 (2000)

Interlayer coupling in DWNTs III

The tunneling matrix elements

$$t_{ij} = t_0 e^{-d_{ij}/a_t},$$

$$A = (R_a \cos v_a / R_a, R_a \sin v_a / R_a, u_a),$$

$$B = (R_b \cos v_b / R_b, R_b \sin v_b / R_b, u_b)$$

with $a_t \sim 0.5 \text{ Å} \ (a_0 = 1.421 \text{ Å})$



$$d_{ij} = \sqrt{(R_a - R_b)^2 + 4R_a R_b \sin^2\left(\frac{v_a}{2R_a} - \frac{v_b}{2R_b}\right) + (u_a - u_b)^2}$$
$$\approx \Delta + \frac{R_a R_b}{2\Delta} \left(\frac{v_a}{R_a} - \frac{v_b}{R_b}\right)^2 + \frac{(u_a - u_b)^2}{2\Delta},$$

with $\Delta = |R_a - R_b| \sim 3.4 \,\text{\AA}$

Interlayer coupling in DWNTs IV

Then the tunneling matrix element

$$t_{ai,bj} = t_0 \exp\left(-\frac{\Delta}{a_t} + \frac{R_a R_b}{2\Delta a_t} \left(\frac{v_a}{R_a} - \frac{v_b}{R_b}\right)^2 + \frac{(u_a - u_b)^2}{2\Delta a_t}\right)$$

In k-space

$$t_{\mathbf{k}_x,\mathbf{k}_y} = t_G \exp\left(\frac{-\Delta a_t}{8R_a R_b} \left(k_{va} R_a + k_{vb} R_b\right)^2\right) \exp\left(\frac{-\Delta a_t (k_{ua} + k_{ub})^2}{8}\right) \delta(k_{va} R_a - k_{vb} R_b) \delta(k_{ua} - k_{ub})$$

$$\cdot \exp\left(\frac{-\Delta a_t (k_{ua} + k_{ub})^2}{8}\right) \delta(k_{va} R_a - k_{vb} R_b) \delta(k_{ua} - k_{ub})$$

with

$$t_G = C \exp\left(-\frac{d}{a_t}\right) \exp\left(-\frac{da_t}{2}|K_0|^2\right) \sim 0.1 \,\mathrm{eV} \qquad d = 3.4 \,\mathrm{\AA}$$

Electronic structure of DWNTs

Two δ functions

$$\delta(k_{va}R_a - k_{vb}R_b)\delta(k_{ua} - k_{ub}) \implies k_{va}R_a - k_{vb}R_b = 0, \quad k_{ua} - k_{ub} = 0$$
 and

$$k_{va}R_a = \ell_a, \quad k_{vb}R_b = \ell_b, \qquad \ell_a, \ell_b = \text{Integer} \qquad \Rightarrow \qquad \ell_a = \ell_b$$

DWNTs with two armchair walls

$$\ell_a = \ell_b = 0 \qquad \Rightarrow \qquad t_{\mathbf{k}_i, \mathbf{k}_j} \neq 0$$

Other DWNTs

$$\ell_a \neq \ell_b \qquad \Rightarrow \qquad t_{\mathbf{k}_i,\mathbf{k}_i} = 0$$

Electronic structure of DWNTs with two armchair walls



DWNTs as Luttinger liquid I

16 new Bosonic operators (i index for two walls)

$$\phi_{c+i} = \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} r\varphi_{r\alpha\sigma i}, \qquad \qquad \Theta_{c+i} = \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} \varphi_{r\alpha\sigma i}, \\ \phi_{c-i} = \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} r\alpha\varphi_{r\alpha\sigma i}, \qquad \qquad \Theta_{c-i} = \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} \alpha\varphi_{r\alpha\sigma i}, \\ \phi_{s+i} = \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} r\sigma\varphi_{r\alpha\sigma i}, \qquad \qquad \Theta_{s+i} = \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} \sigma\varphi_{r\alpha\sigma i}, \\ \phi_{s-i} = \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} r\alpha\sigma\varphi_{r\alpha\sigma i}, \qquad \qquad \Theta_{s-i} = \frac{1}{4\sqrt{\pi}} \sum_{r\alpha\sigma} \alpha\sigma\varphi_{r\alpha\sigma i}$$

The field operator

$$\varphi_{r\alpha\sigma i} = \frac{\sqrt{\pi}}{2} (r\phi_{c+i} + r\alpha\phi_{c-i} + r\sigma\phi_{s+i} + r\alpha\sigma\phi_{s-i} + \Theta_{c+i} + \alpha\Theta_{c-i} + \sigma\Theta_{s+i} + \alpha\sigma\Theta_{s-i})$$

DWNTs as Luttinger liquids II

Coulomb interaction is

$$H_{I} = \frac{1}{2} \sum_{\sigma \sigma'} \int d\mathbf{r} d\mathbf{r}' \Psi_{\sigma}^{\dagger}(\mathbf{r}) \Psi_{\sigma'}^{\dagger}(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \Psi_{\sigma'}(\mathbf{r}') \Psi_{\sigma}(\mathbf{r}).$$

Forward scattering in a wall

$$H_{\alpha FS}^{(0)} = \sum_{i} \frac{1}{2} \int dx dx' \ \rho_i(x) V_i(x - x') \rho_i(x'),$$

Forward scattering between walls

$$H_{\alpha FS}^{\prime(0)} = \frac{1}{2} \int dx dx' \ \rho_1(x) V_{12}(x - x') \rho_2(x'),$$

DWNTs as Luttinger liquids III

The Hamiltonian is

$$H_{0} + H_{\alpha FS}^{(0)} + H_{\alpha FS}^{\prime(0)} = \sum_{j\delta i} \int \frac{dk}{2\pi} \frac{\hbar v_{j\delta i}}{2} \left(\Pi_{j\delta i}(k) \Pi_{j\delta i}(-k) + k^{2} \phi_{j\delta i}(k) \phi_{j\delta i}(-k) \right) \\ + \sum_{il} \int \frac{dk}{2\pi} \frac{4k^{2} V_{il}(k)}{\pi} \phi_{c+i}(k) \phi_{c+l}(-k)$$

Coulomb interaction only affect $(c + \pm)$ modes.

$$\frac{\hbar v_{c+\pm}' K_{c+\pm}'}{2} = \frac{\hbar v}{2}, \ \frac{\hbar v_{c+\pm}'}{2K_{c+\pm}'} = \frac{\hbar v}{2} \left(1 + \frac{2(V_1 + V_2)}{\hbar \pi v} \pm \sqrt{\left(\frac{2(V_1 - V_2)}{\hbar \pi v}\right)^2 + \left(\frac{4V_{12}^2}{\hbar \pi v}\right)^2} \right)^2 + \left(\frac{4V_{12}^2}{\hbar \pi v}\right)^2 \right)^2$$

 $v_{j\delta i} = v, \qquad K_{j\delta i} = 1, \qquad \text{Other modes}$ Double wall nanotubes are Luttinger liquids!

Tunneling density of states

Tunneling density of states (TDOS) is

$$\rho(\epsilon, x) = \frac{1}{2\pi\hbar} dt \, e^{-i\epsilon t/\hbar} \langle \psi^{\dagger}(x, t)\psi(x, 0) \rangle$$

$$\rho(\epsilon) \sim (kT)^{\alpha} \cosh\left(\frac{\epsilon}{2kT}\right) \left|\Gamma\left(\frac{1}{2}(1+\alpha) + i\frac{\epsilon}{2\pi kT}\right)\right|^2$$

$$\rho_{\rm end}(\epsilon) \sim \epsilon^{\alpha_{end}}, \qquad \rho_{\rm bulk}(\epsilon) \sim \epsilon^{\alpha_{bulk}} \qquad T \to 0$$

The current is given as

$$I \propto \int_0^V d\epsilon \,\rho_1(\epsilon)\rho_2(\epsilon) \quad \Rightarrow \quad \frac{dI}{dV} \propto \rho_1(\epsilon)\rho_2(\epsilon)$$



Tunneling density of state of DWNT

The exponents of a DWNT — only out wall is connected to leads

$$\alpha_{\text{end,out}} = \frac{1}{4} \sin^2 \xi \left(\frac{1}{K'_{c++}} - 1 \right) + \frac{1}{4} \cos^2 \xi \left(\frac{1}{K'_{c+-}} - 1 \right),$$

$$\alpha_{\text{bulk,out}} = \frac{1}{8} \sin^2 \xi \left(K'_{c++} + \frac{1}{K'_{c++}} - 2 \right) + \frac{1}{8} \cos^2 \xi \left(K'_{c+-} + \frac{1}{K'_{c+-}} - 2 \right),$$

For examples

$$\alpha_{\text{end,out}} = 1.033, \qquad \alpha_{\text{bulk,out}} = 0.429 \qquad (5,5)@(10,10)$$

 $\alpha_{\text{end,out}} = 1.254, \qquad \alpha_{\text{bulk,out}} = 0.523 \qquad (10,10)$

Summary and outlook

- No interlayer coupling in DWNTs except those with two armchair walls
- Most DWNTs can be described as two Luttinger liquids coupled by Coulomb interaction
- The conductance has power law dependence on applied voltage. Exponents decrease in DWNTs.

To be continued

• DWNTs with interlayer tunneling, disorder, . . .