# Electron-electron interactions in carbon nanotubes

Reinhold Egger
Institut für Theoretische Physik
Heinrich-Heine-Universität
Düsseldorf, Germany

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# Overview

Three lectures:

1. Effective field theory and phase diagram of SWNTs

2. Charge and spin transport in SWNTs

3. More complexity: Crossed tubes and intrinsic Coulomb blockade in MWNTs

# Classification

- Multi-wall nanotubes (MWNTs)
  $\Rightarrow$ several (typically ten) concentrically arranged graphite sheets (“Russian doll”), typical dimensions:
  $L \approx \mu$m to mm, $R \approx 5$ nm

  Schönenberger et al., Appl. Phys. A 69, 283 (1999)

- Ropes of single-wall nanotubes (SWNTs), triangular lattice of 5-100 SWNTs

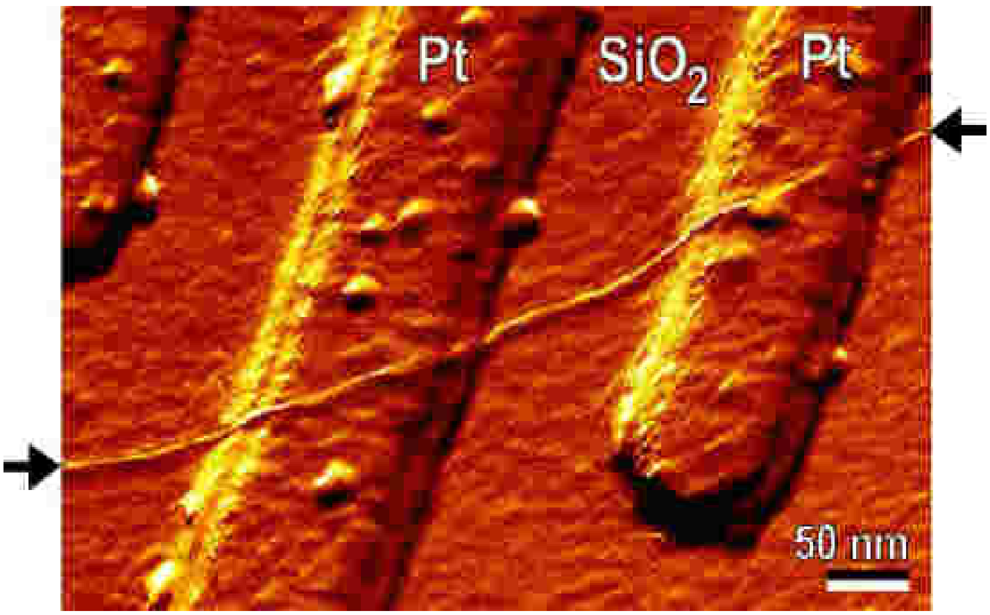
  Bockrath et al., Nature 397, 598 (1999)

- Individual SWNT, typical dimensions:
  $L \approx 1\mu$m, $R \approx 1$ nm

  Yao et al., Nature 402, 273 (1999)

AFM image of SWNT ($L \approx 3\mu$m, $R \approx 1.4$ nm):

Tans et al., Nature 386, 474 (1997)



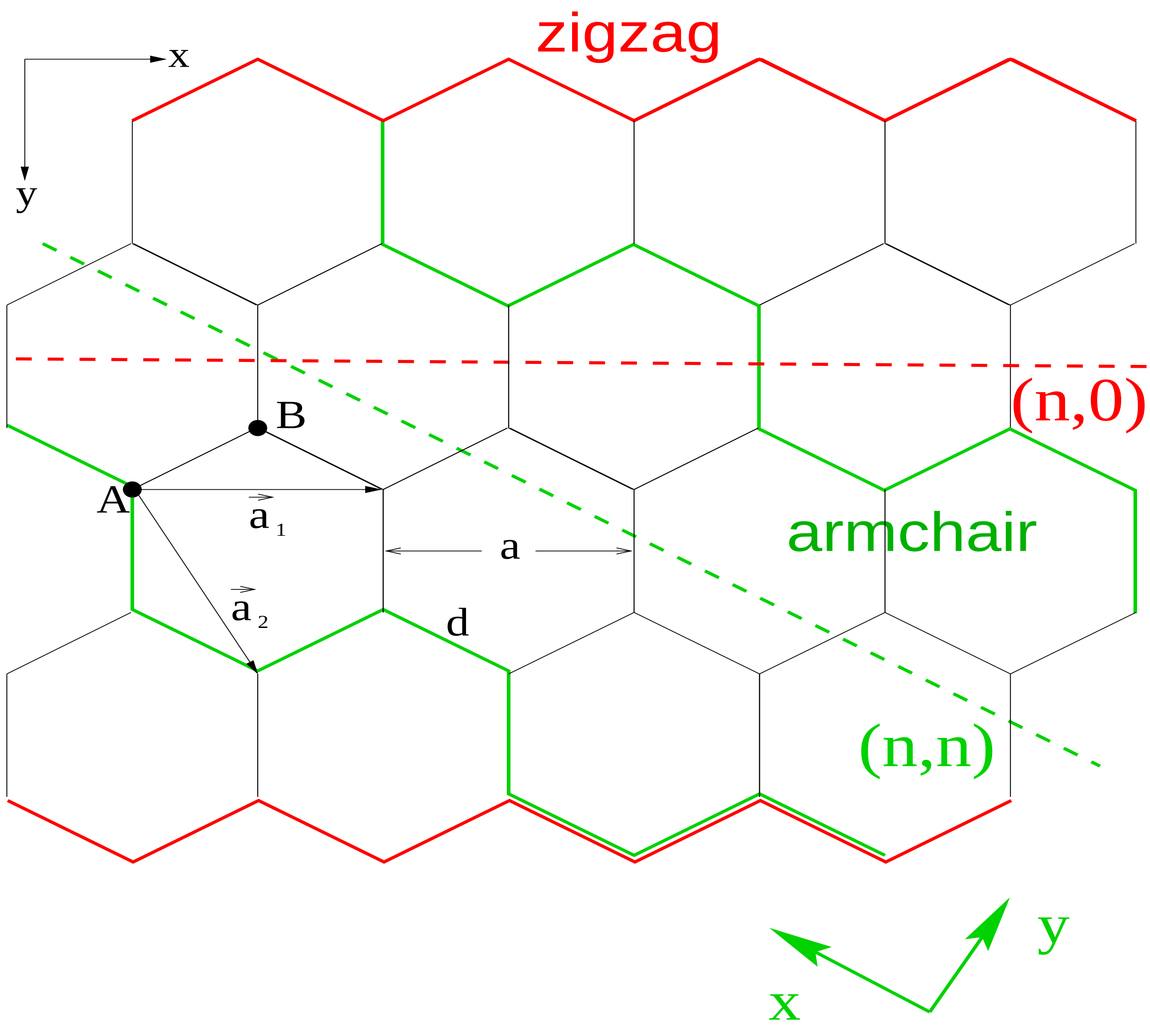

Fermi (doping) level tunable, e.g. using gate voltage

$\Rightarrow$ Transport experiments for individual nanotubes

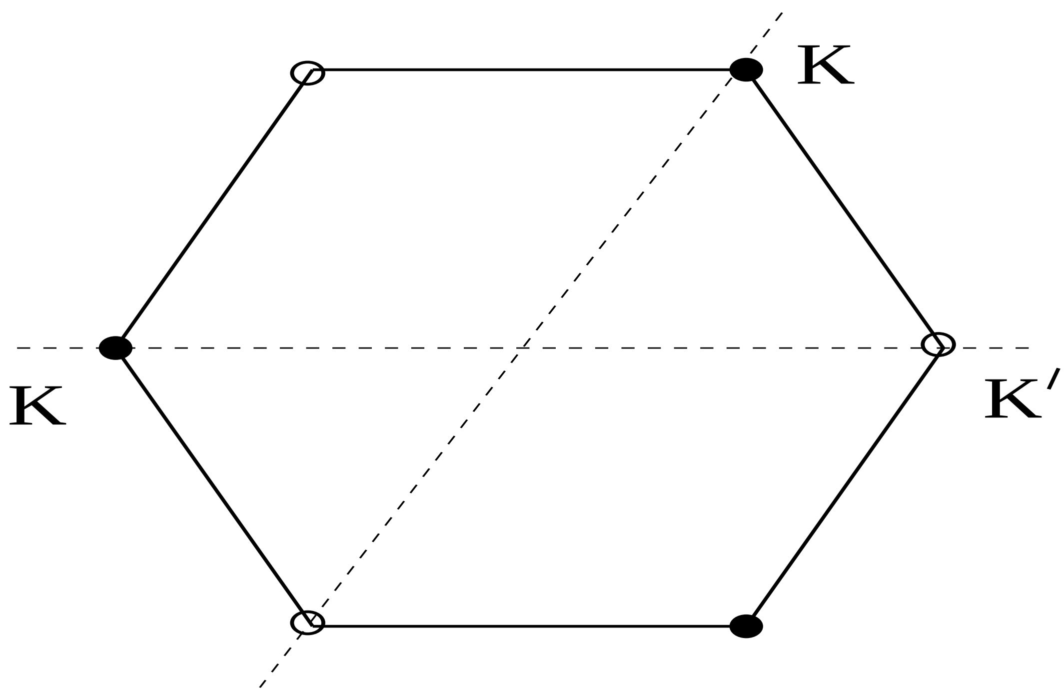
$\Rightarrow$ What has theory to say about this?

# 2D graphite sheet

Basis contains two atoms $(a = \sqrt{3}d, d = 1.42\text{Å})$



First Brillouin zone = Hexagon




Note: exactly two independent corner points $K, K'$

Band structure from simple nearest-neighbor tight binding approach

- Valence band and conduction band touch only at isolated corner points with $E = 0$

- For each C one $\pi$ electron $\Rightarrow E_F = 0$
$\Rightarrow$ no closed Fermi surface, only isolated Fermi points

- Close to $K$ points, relativistic dispersion (light cone)

$$E(\vec{q}) = v_F |\vec{q}| \ , \quad \vec{q} = \vec{k} - \vec{K}$$

# Nanotube
## = rolled graphite sheet

- $(n, m)$ nanotube for superlattice vector

$$\vec{T} = n\vec{a}_1 + m\vec{a}_2$$

- Transverse component of wavevector is quantized:

$$\vec{T} \cdot \vec{k}/2\pi = \text{integer}$$

- Nanotube metallic only if Fermivector obeys this condition ⇒ holds for

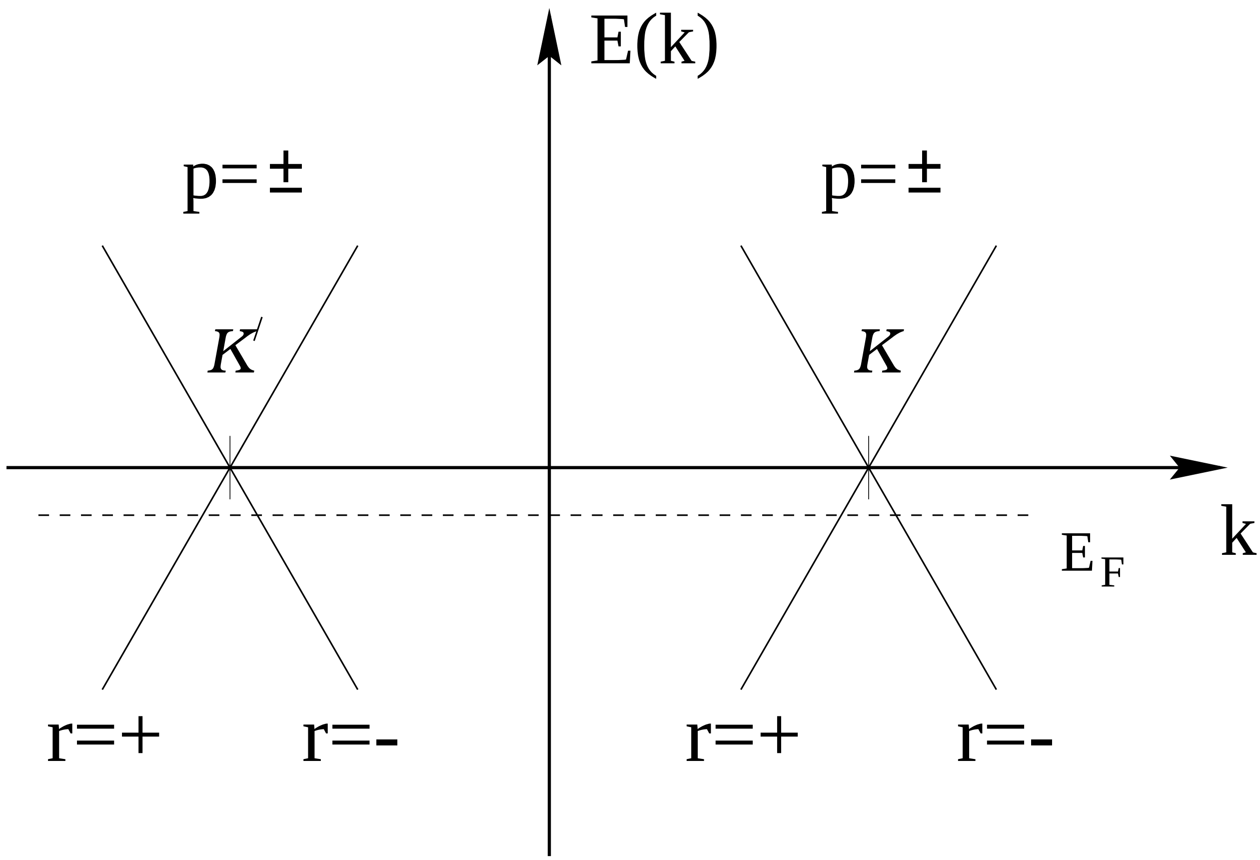
$$(2n + m)/3 = \text{integer}$$

experimentally verified!

- otherwise insulator with band gap $\approx 1$ eV

Helicity ⇒ electronic properties

# Metallic SWNT: Dispersion relation




Basis of graphite sheet contains 2 atoms
$\Rightarrow$ two sublattices $p = \pm \Leftrightarrow R/L$
$\Rightarrow$ two degenerate Bloch waves $\phi_{p\alpha}(x, y)$
at each Fermi point $\alpha = \pm$

# SWNT = 1D ballistic quantum wire

Tans et al., Nature 386, 474 (1997)

- Transverse momentum quantization ($k_y = 0$) $\Rightarrow$ 1D quantum wire with only 2 bands intersecting the Fermi energy, all other bands are $> 1eV$ away and can be ignored at low energy scales

- Massless 1D Dirac Hamiltonian on energy scales $< 1eV$ (even at room temperature)

- $E_F \neq 0$ due to doping or gate electrodes

- Two distinct momenta for backscattering: $k_F$ from Fermi point and $q_F = |E_F|/v_F$ from doping

# Breakdown of Fermi liquid in 1D

- In 1D quasiparticles unstable because of electron-electron interactions

- Reduced phase space

- Stable excitations: collective electron-hole pair modes ("plasmons")

- Often leads to Luttinger liquid

  Luttinger, J.Math.Phys. 4, 1154 (1963)

  Haldane, J.Phys.C 14, 2585 (1981)

- Examples: nanotubes, quantum wires, FQH edge states, long chain molecules

- Gaussian field theory $\Rightarrow$ exactly solvable!

# Bosonization approach

Collective electron-hole excitations $\Rightarrow$ bosonic plasmon phase field $\varphi(x)$

Massless Dirac Hamiltonian $\Rightarrow$
Harmonic chain problem

$$H_0 = \frac{v_F}{2} \int dx \left( \Pi^2(x) + (\partial_x \varphi(x))^2 \right)$$

Kronig (1935)

Express also Fermion operator via $\varphi(x)$:

$$\psi^\dagger_{R/L}(x) \propto \exp\left( \pm i[k_F x + \varphi(x)] + i \int^x dx' \Pi(x') \right)$$

$\Rightarrow$ transform interacting 1D model into equivalent bosonic model

Electron density operator:

$$\rho(x) = \partial_x \varphi + \frac{k_F}{\pi} \cos[2k_F x + 2\varphi]$$

# Coulomb interaction

Within the 1D conductor, interaction potential $U(x-x')$ is typically externally screened by gate in a distance $d$

$$U(x-x') \approx \frac{e^2}{|x-x'|} - \frac{e^2}{\sqrt{(x-x')^2+4d^2}}$$

$\Rightarrow$ effectively short-ranged for $|x-x'| > d$

Simple description for long lengthscales: retain only $k=0$ Fourier component $U_0$

$\Rightarrow$ interaction strength is just a single dimensionless parameter:

$$g = \frac{1}{\sqrt{1+U_0/\pi v_F}} \leq 1$$

Bosonization also works for unscreened case, since only weak logarithmic divergence
$\Rightarrow$ multiplicative logarithmic corrections to Luttinger power laws

# Luttinger liquid

Coulomb interaction is density-density interaction
$\Rightarrow$ keeping only "slow" component $\rho \sim \partial_x \varphi$ corresponding to forward scattering gives

## Luttinger liquid Hamiltonian

$$H = \frac{v_F}{2} \int dx \left( \Pi^2(x) + (1/g^2)(\partial_x \varphi(x))^2 \right)$$

$\Rightarrow$ exactly solvable Gaussian field theory

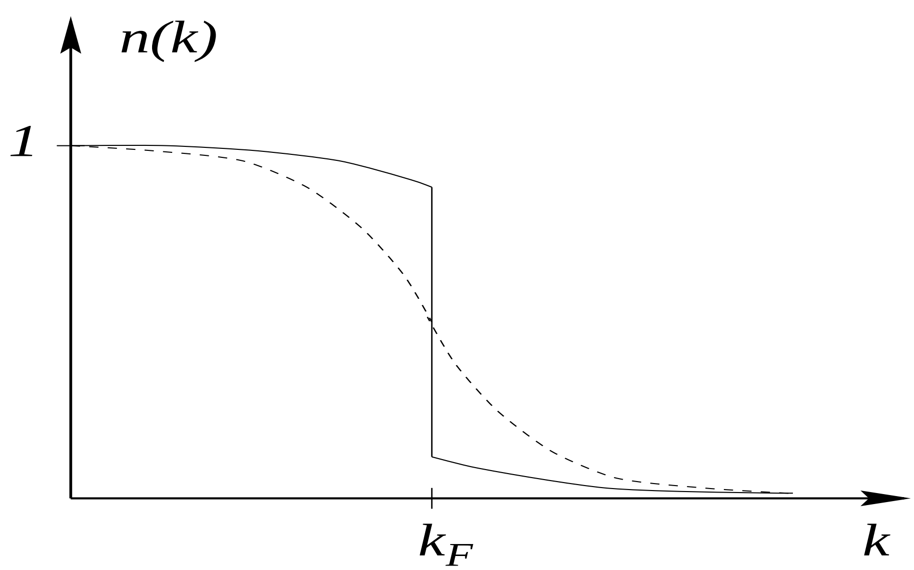
"Fast" component corresponds to electron-electron backscattering $\Rightarrow$ ignored in Luttinger model, but often irrelevant

# Luttinger liquid properties

Electron distribution function:
smeared Fermi surface $(T = 0)$

$$n_k \propto |k - k_F|^{\alpha} \quad \text{for} \quad k \to k_F$$

$$\alpha = (g + 1/g - 2)/4$$

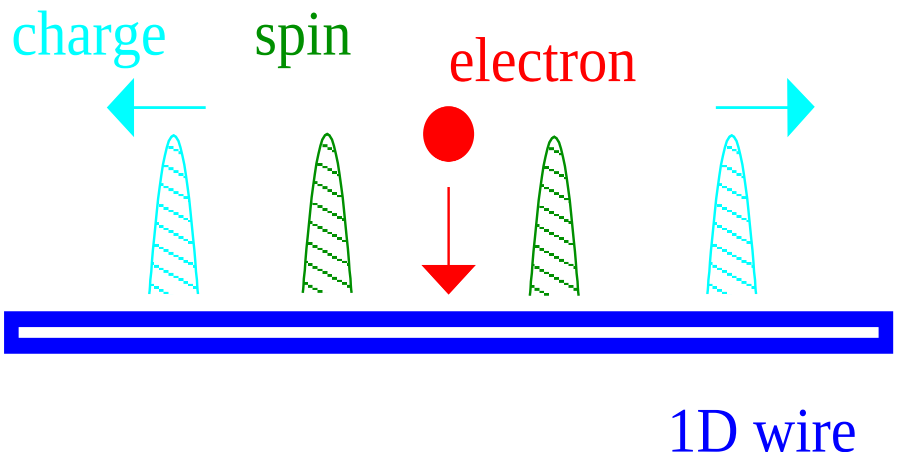


- Tunneling conductance into Luttinger liquid power-law suppressed $G \propto T^{\eta/2}$ with geometry-dependent exponents

$$\eta_{\text{end}} = (1/g - 1)/2 > 2\eta_{\text{bulk}}$$

- Electron fractionalizes into spinons and holons (solitons of Gaussian theory)

# Spin charge separation




- Additional electron decays into spin and charge wave packets

- Both wave packets decouple and propagate with different velocities:

$$v_{\text{spin}} \neq v_{\text{charge}}$$

- Spatial separation of electronic spin and charge degrees of freedom

- So far no unambiguous experimental observation!

# Low-energy theory for metallic SWNT

Low-energy expansion of electron operator using Bloch waves

$$\phi_{p\alpha}(x,y) = \frac{1}{\sqrt{2\pi R}} \exp(-i\alpha\vec{K}\vec{r})$$

sublattice $p = \pm$ and Fermi point $\alpha = \pm$

- Quantized transverse momentum implies orbital contribution $\sim \exp(imy/R)$

- All $m \neq 0$ states cost energy $\geq \hbar v_F/R \approx 1\ eV \Rightarrow$ keep only $m = 0$

- Then: two spindegenerate copies of 1D massless Dirac Hamiltonian

- Perfectly contacted SWNT has conductance $4e^2/h$

Resulting expansion for electron operator

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

$\Rightarrow$ 1D Fermions $\psi_{p\alpha\sigma}(x)$ for spin $\sigma = \pm$

Central question:

Does long-ranged Coulomb interaction result in Luttinger liquid or more exotic non-Fermi liquid? (assume individual tube on insulating substrate)

Egger & Gogolin, PRL 79, 5082 (1997)

EPJB 3, 281 (1998)

Kane, Balents & Fisher, PRL 79, 5086 (1997)

# Coulomb interaction

On the tube surface, Coulomb interaction potential $U(\vec{r}-\vec{r}\,')$ is

$$\frac{e^2/\kappa}{\sqrt{(x-x')^2+4R^2\sin^2[(y-y')/2R]+a_z^2}}$$

with dielectric constant $\kappa$ and $a_z \approx a$

Second-quantized interaction Hamiltonian

$$\begin{aligned} H_I &= \frac{1}{2}\sum_{\sigma\sigma'}\int d\vec{r}\int d\vec{r}\,'\,\Psi^\dagger_\sigma(\vec{r})\Psi^\dagger_{\sigma'}(\vec{r}\,') \\ &\times U(\vec{r}-\vec{r}\,')\Psi_{\sigma'}(\vec{r}\,')\Psi_\sigma(\vec{r}) \end{aligned}$$

Now insert expansion for $\Psi$
$\Rightarrow$ messy 1D model

# 1D Coulomb interaction

Momentum conservation ⇒ only allowed interaction processes off half-filling:

- Forward scattering

  Small momentum exchange, couples "slow" 1D densities. Physically due to long-range part of interaction.

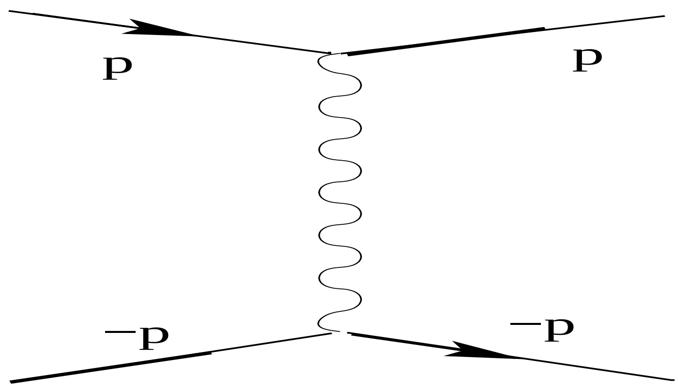
- Backscattering

  Large momentum exchange, couples "fast" 1D densities. Physically due to short-range interactions.

  Backscattering couplings scale $\sim 1/R$ ⇒ could be very large in ultrathin SWNTs, but small in "normal" SWNTs.

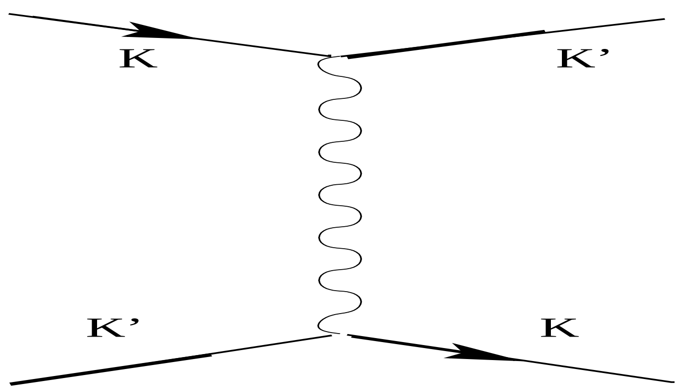
# Backscattering couplings

- Momentum exchange $2q_F$




Coupling constant $f/a \approx 0.05e^2/R$

- Momentum exchange $2k_F$




Coupling constant $b/a \approx 0.1e^2/R$

# Bosonization

4 bosonic phase fields $\varphi_a(x)$ with $a = c+, c-, s+, s-$, and $\Pi_a = -\partial_x \theta_a$

$c/s$: Charge/spin degrees of freedom
$\pm$: Symmetric/antisymmetric combinations of Fermi points

Bosonized Hamiltonian
= Luttinger liquid plus nonlinearities

$$
\begin{aligned}
H &= \frac{v_F}{2} \int dx \sum_a \left[ \Pi_a^2 + g_a^{-2} (\partial_x \varphi_a)^2 \right] \\
&+ f \int dx [- \cos\varphi_{c-} \cos\varphi_{s-} - \cos\varphi_{c-} \cos\varphi_{s+} \\
&\qquad + \cos\varphi_{s-} \cos\varphi_{s+}] \\
&+ b \int dx \cos\varphi_{c-} [\cos\varphi_{s-} + \cos\theta_{s-}]
\end{aligned}
$$

Electron-electron interaction and tube radius determine couplings $f, b, g_a$

$$g_a \simeq 1 \quad \text{except} \quad g_{c+} = g$$

# Luttinger parameter

Estimate for unscreened interactions shows log divergence
$\Rightarrow$ natural cutoff is tube length $L$:

$$g = \left(1 + \frac{8e^2}{\pi\kappa\hbar v_F} \ln[L/2\pi R]\right)^{-1/2}$$
$$= \left(1 + \frac{2E_c}{\Delta}\right)^{-1/2}$$

with charging energy $E_c$ and level spacing $\Delta$

Estimate depends only weakly on $L, R$
$\Rightarrow$ for typical parameters

$$g \approx 0.2 \text{ to } 0.3$$

$\Rightarrow$ very strong correlations

# Nonlinearities?

- Total charge $(a = c+)$ channel decouples $\Rightarrow$ perturbative renormalization group analysis can be applied

- $b$ is marginally relevant $\Rightarrow$ destroys Luttinger liquid behavior for $E \to 0$

- $f$ is first marginally irrelevant, but becomes relevant around new fixed point

Analytical solution via
Majorana refermionization

$\Rightarrow$ complete characterization of non-Fermi liquid state in SWNTs

# Majorana refermionization

$f$ marginally irrelevant, but $b$ relevant
$\Rightarrow$ start with $f = 0$

- Nonlinearity acts only in $(c-, s-)$ sector

- Define new "effective" 1D Fermions for $a = (c-, s-)$

$$\psi_{a,R/L}(x) \sim \exp[-(i/2)(\pm\theta_a(x) + \varphi_a(x))]$$

- Express (complex) Dirac Fermions in terms of (real) Majorana Fermions

$$\begin{aligned} \psi_{s-,R/L} &= [\xi_{1,R/L}(x) + i\xi_{2,R/L}(x)]/\sqrt{2} \\ \psi_{c-,R/L} &= [\xi_{3,R/L}(x) + i\xi_{4,R/L}(x)]/\sqrt{2} \end{aligned}$$

Resulting Majorana Hamiltonian for $(c-, s-)$ sector:

$$H = \frac{-iv_F}{2} \sum_{j=1}^{4} \int dx(\xi_{jR}\partial_x\xi_{jR} - \xi_{jL}\partial_x\xi_{jL}) + 2b \int dx(\xi_{3R}\xi_{3L} + \xi_{4R}\xi_{4L})\xi_{1R}\xi_{1L}$$

$\Rightarrow \xi_2$ stays massless, but $\xi_{1,3,4}$ become massive (gapped)

Majorana mean field theory yields energy gap for $\xi_{1,3,4}$ with bandwidth $D$

$$k_B T_b = D \exp[-\pi v_F/\sqrt{2}\, b]$$

$\Rightarrow (c-)$ channel massive, but $(s-)$?

Bosonized version: Uncertainty relation prevents pinning of $\varphi_{s-}$ or $\theta_{s-}$

Effective Hamiltonian for $(s-)$ channel:

$$H_{s-} = H_1[\xi_1] + H_2[\xi_2]$$

$$\begin{aligned} H_j[\xi_j] &= \frac{-iv_F}{2}\int dx(\xi_{jR}\partial_x\xi_{jR} - \xi_{jL}\partial_x\xi_{jL}) \\ &- im_j\int dx\ \xi_{jR}\xi_{jL} \end{aligned}$$

with $m_1 = m_b$ and $m_2 = 0$
$\Rightarrow$ Mapping to two classical 2D Ising models $I_{1,2}$, with $I_1$ disordered $(T > T_c)$ and $I_2$ critical $(T = T_c)$
$\Rightarrow$ take exact solution for 2D Ising

$f \neq 0$ can also be treated via Majorana refermionization, opens gap

$$T_f = (f/b)T_b \leq T_b$$

in spin channels $(s+, s-)$

# Three temperature regimes

1. High-temperature regime: all fields are massless

   Luttinger liquid

   (even at room temperature)

2. Intermediate temperatures ($T_f < T < T_b$) $\Rightarrow$ ($c-$) massive, ($s-$) in universality class of classical 2D Ising model

3. $T < T_f$ $\Rightarrow$ all fields gapped except $\varphi_{c+}$

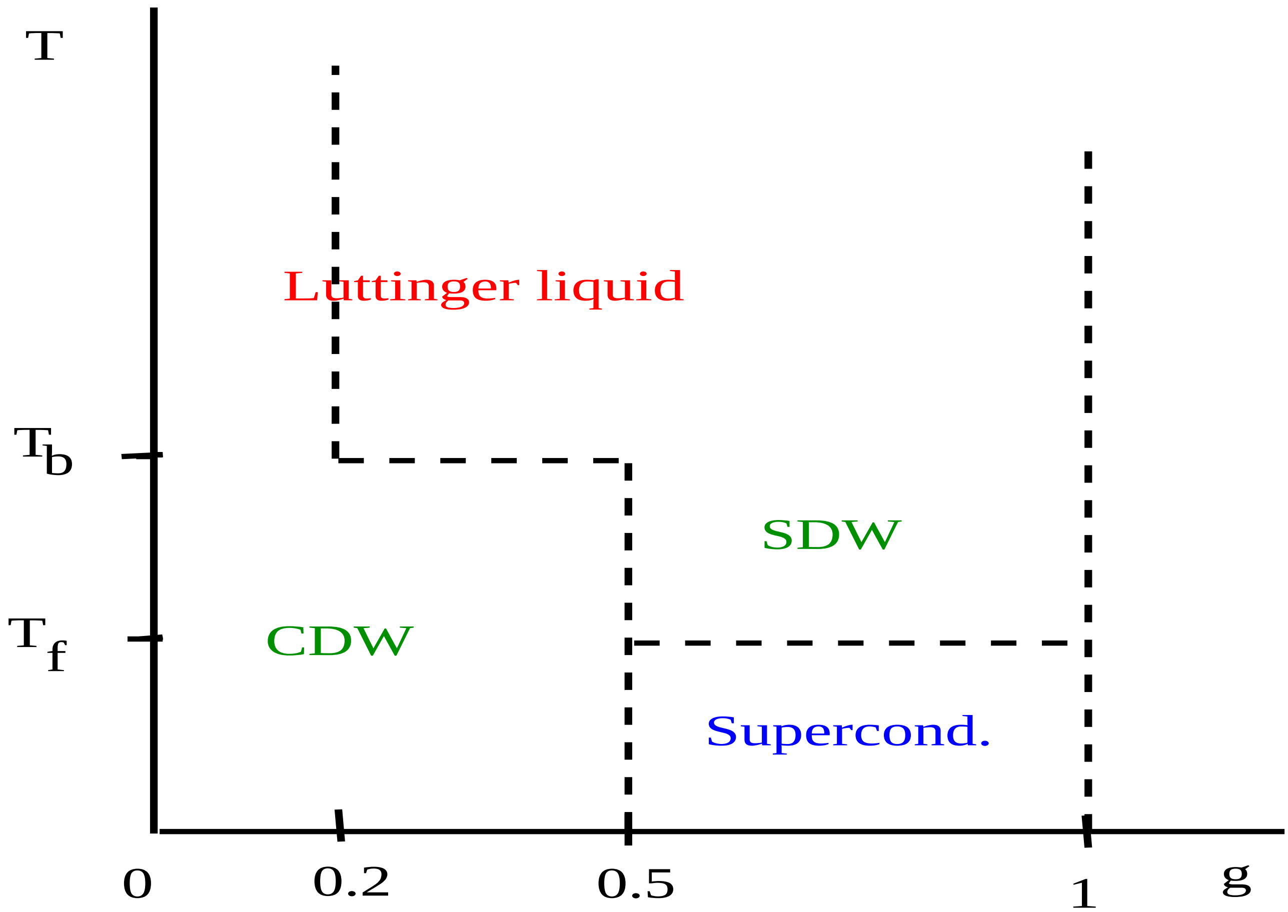
Estimate for $R = 1.4$ nm

$$T_f \leq T_b \approx 0.1 \text{ mK}$$

$\Rightarrow$ in practice Luttinger liquid

But: Low-temperature phases important for ultrathin tubes!

# Phase diagram




no real order, but slow algebraic power law decay!

# 1D Superconductivity

Existence of strong intrinsic superconducting fluctuations in ultrathin SWNTs ($R = 2$ Å) experimentally detected

Tang et al., Science 292, 2462 (2001)

Proposed mechanism: Cooper pair formation is triggered by repulsive interactions, analogous to d-wave superconductivity in two-leg Hubbard ladders

Egger & Gogolin, PRL 79, 5082 (1997)

Gonzalez, PRL 87, 136401 (2001)

# Tunneling DOS

Tunneling density of states:

$$\nu(x,E) \sim \int_0^\infty dt \; e^{iEt}\langle\psi(x,t)\psi^\dagger(x,0)\rangle$$

Electron is not a good excitation
$\Rightarrow$ decomposes into plasmon modes
$\Rightarrow$ orthogonality catastrophe,
with power-law scaling

$$\langle\psi(x,t)\psi^\dagger(x,0)\rangle \sim t^{-1-\eta}$$

Power-law suppression of TDOS:

$$\nu(x,E) \sim E^\eta$$

Exponent $\eta$ depends on geometry. Consider semi-infinite SWNT: $x > 0$

- Bulk exponent for $x \gg v_F/|E|$:

$$\eta_{\text{bulk}} = \frac{(1/g) + g - 2}{4}$$

- End exponent for $x \ll v_F/|E|$:

$$\eta_{\text{end}} = \frac{(1/g) - 1}{2} > 2\eta_{\text{bulk}}$$

- Experimentally verified in SWNTs

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

Yao et al., Nature 402, 273 (1999)

Postma et al., Science 293, 76 (2001)

# Conclusions Lecture 1

- SWNT are ballistic 1D quantum wires with strong interactions

- Phase diagram: superconductivity, charge density wave character at low temperatures, Luttinger liquid at higher temperatures

- Sophisticated field theory methods can be applied to description of a single molecule