

SUMMER SCHOOL
on
LOW-DIMENSIONAL QUANTUM SYSTEMS:
Theory and Experiment
(16 - 27 JULY 2001)

PLUS

PRE-TUTORIAL SESSIONS
(11 - 13 JULY 2001)

SINGLE-WALL CARBON NANOTUBES

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These are preliminary lecture notes, intended only for distribution to participants

Single-wall Carbon Nanotubes

Sasha Gogolin

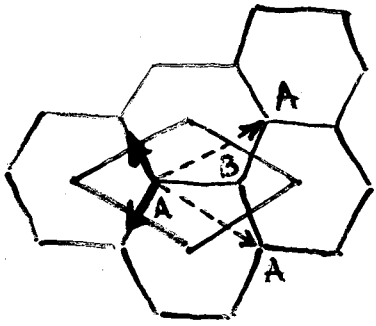
Imperial College London, Math Dept

Collaboration: Egger, Komnik

Plan:

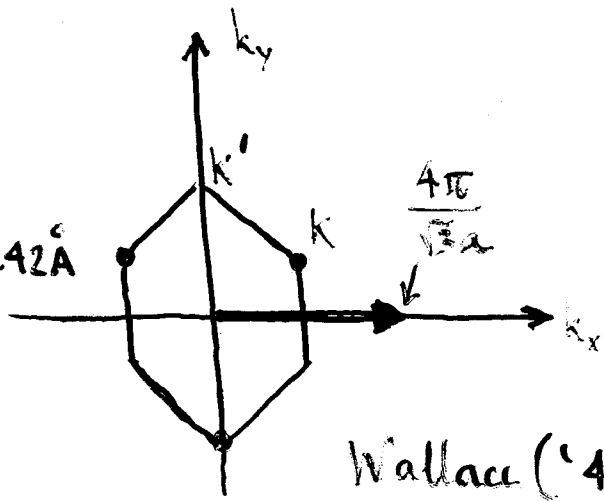
- preliminaries
- making of tubes
- interaction effects
- conductance experiments
- field emission

Graphite



$$[CC] = d = 1.42 \text{ \AA}$$

$$a = \sqrt{3}d$$



Wallace ('47)

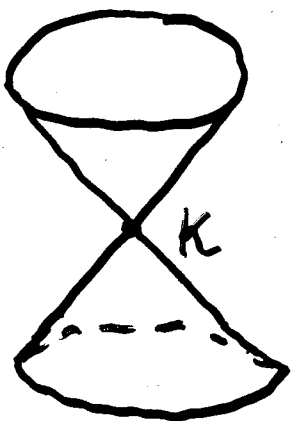
$$\vec{a}_1 = a\hat{x}, \vec{a}_2 = a\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right)$$

$$H = \gamma_0 \sum_{\vec{n}} \left[A_{\vec{n}}^+ B_{\vec{n}} + A_{\vec{n}+\vec{a}_1, n_2}^+ B_{\vec{n}} + A_{\vec{n}_1, n_2+\vec{a}_2}^+ B_{\vec{n}} \right] + \text{H.c.} =$$

$$= \gamma_0 \sum_{\vec{k}} \left[1 + 2e^{i\frac{\sqrt{3}}{2}k_x a} \cos\left(\frac{k_y a}{2}\right) \right] A_{\vec{k}}^+ B_{\vec{k}} + \text{H.c.} \rightarrow \begin{bmatrix} \epsilon & t_{\vec{k}} \\ t_{\vec{k}}^* & 0 \end{bmatrix}$$

$$E_{2D}(\vec{k}) = \pm |t_{\vec{k}}|^2 = \pm \gamma_0 \left\{ 1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right) \right\}^{1/2}$$

Around K-points $\vec{k} = \vec{k} + \vec{q}$ and $E_{2D}(\vec{q}) = \pm v_F |\vec{q}|$



2D Dirac

$$v_F = 10^5 \text{ m/s}$$

Magnetic field $H \perp$ plane

Rammal, J Phys (1985)

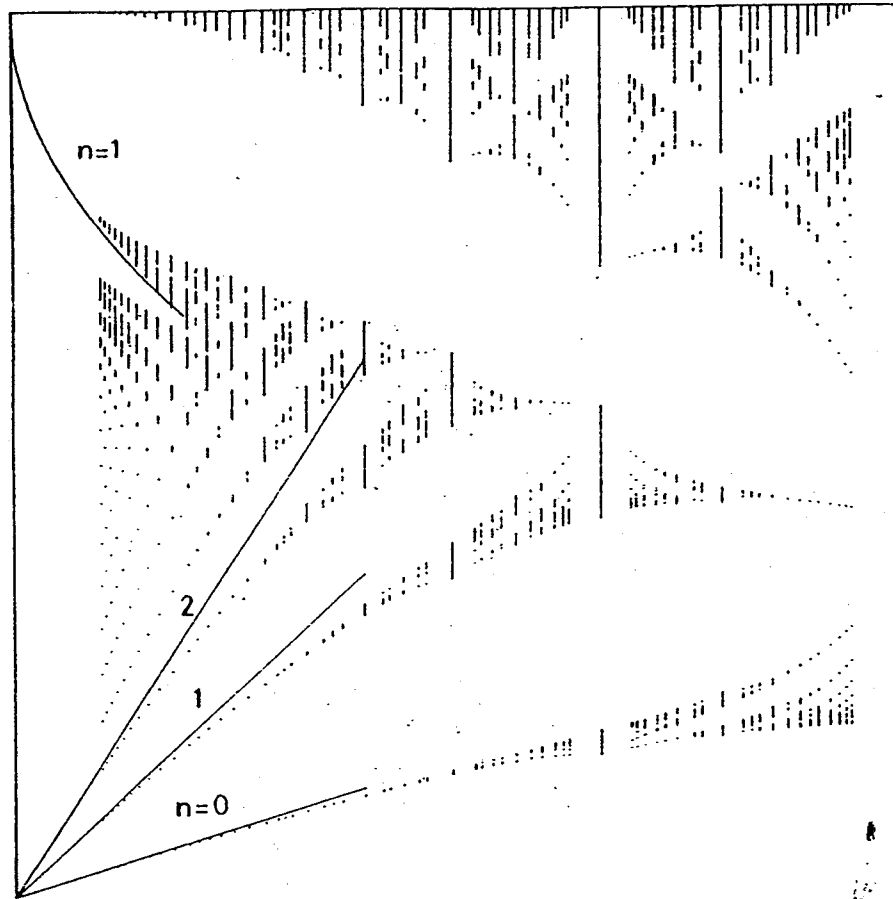


Fig. 4. — Energy spectrum for broadened Landau levels.

Phase factor $\int_{\alpha}^{\beta} \vec{A} d\vec{e}$ $\gamma_{\alpha\beta} = \frac{2\pi}{\phi_0} \int_{\alpha}^{\beta} \vec{A} d\vec{e}$

\Rightarrow difference equations \Rightarrow linearisation around Dirac point

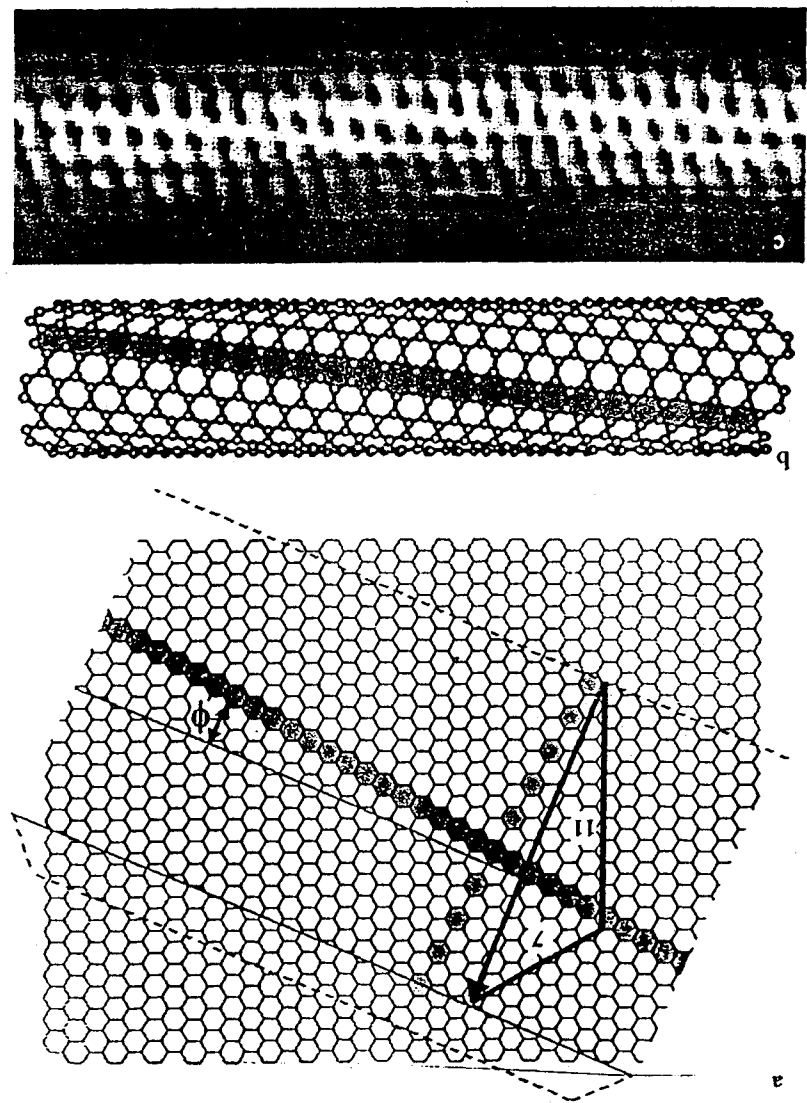
\Rightarrow spectrum: $E^2 \approx \sqrt{3} \gamma h$ (Landau levels)

$h = 1, 2, 3, \dots$

$\gamma = 2\pi \phi / \phi_0, \phi = \frac{3\sqrt{3}}{2} H a_0^2$

energy $k_B T$, about 0.025 eV. Only two one-dimensional subbands cross the energy in metallic nanotubes; all the through such tubes is therefore predicted by only this pair of subbands. Because each subband can in principle support a conductance of $G_0 = 2e^2/h$ (Adapted from Wilder *et al.*, ref. 6.)

FIGURE 1. HOW TO WRAP A NANOTUBE
 a single sheet of graphite. First, copy the part (a) onto a transparent overhead sheet. Second, cut out the part of the sheet indicated by the dashed lines. Third, fold up the part so that the blue arrow's tail coincide with its head. Match the hexagons on the overlapped carefully to those on the tube body. Finally, fasten the tube together with transparent tape. A nanotube with indices (11,7) now has been formed. The indices describe the projection of the circumference of the sheet onto the basis vector of the graphite lattice, as shown. The red arrow illustrates the winding of hexagons along the tube direction. It forms the angle ϕ (the tube angle) with respect to the tube axis. Wrapping the sheet along the yellow or green hexagonal rows instead of along the blue vector leads to (n,0) "zigzag" tubes (so named because of rows of alternating carbon bonds around circumference) or (m,m) "armchair" tubes (circumference) parallel to the tube axis, respectively. The indices (m,m) are crucially important for the electronic properties of nanotubes: Tubes for which $n - m = 3i$, i an integer, are metallic; all others are semiconducting. (b) Atomic structure of a nanotube that results from the folding above (image courtesy of Philippe Lambin, University of Namur). (c) Atomically resolved scanning tunneling microscope image of a nanotube (Adapted from Wilder *et al.*, ref. 6.)



GRAPHENE TUBULES BASED ON C_{60}

$$k_x = \frac{h}{\lambda} = \frac{2\pi}{\lambda}$$

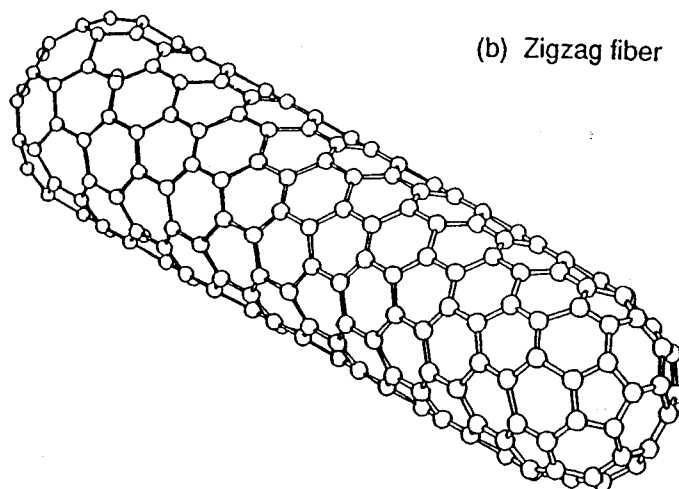
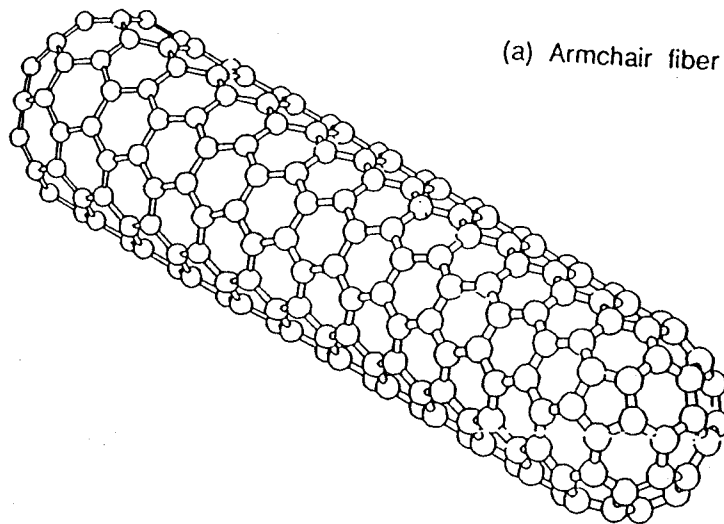
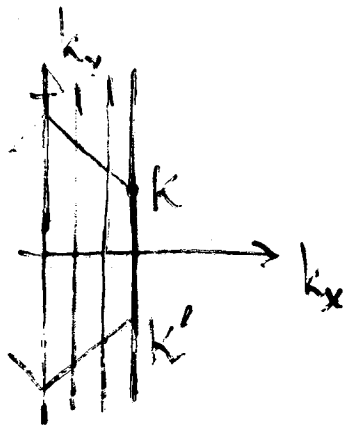


FIG. 2. Atomic arrangements of carbon atoms in the (a) armchair fiber and (b) zigzag fiber.

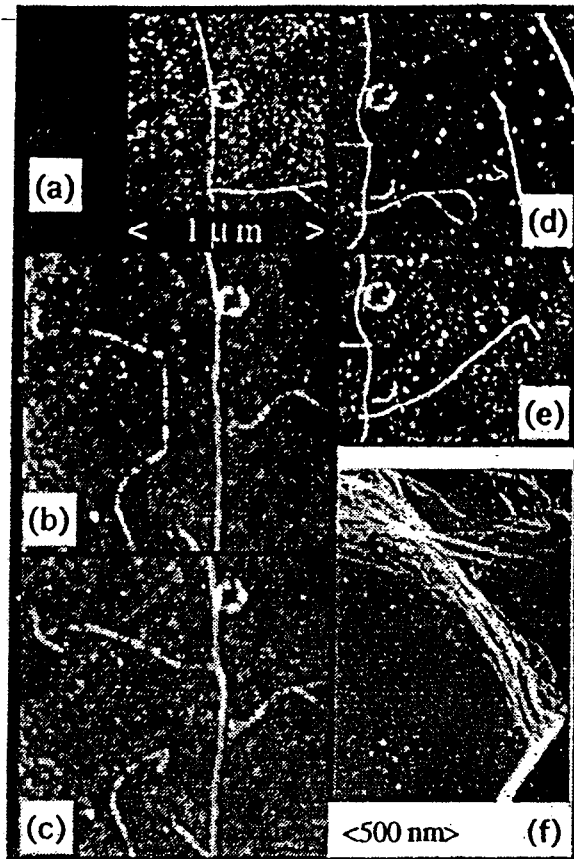
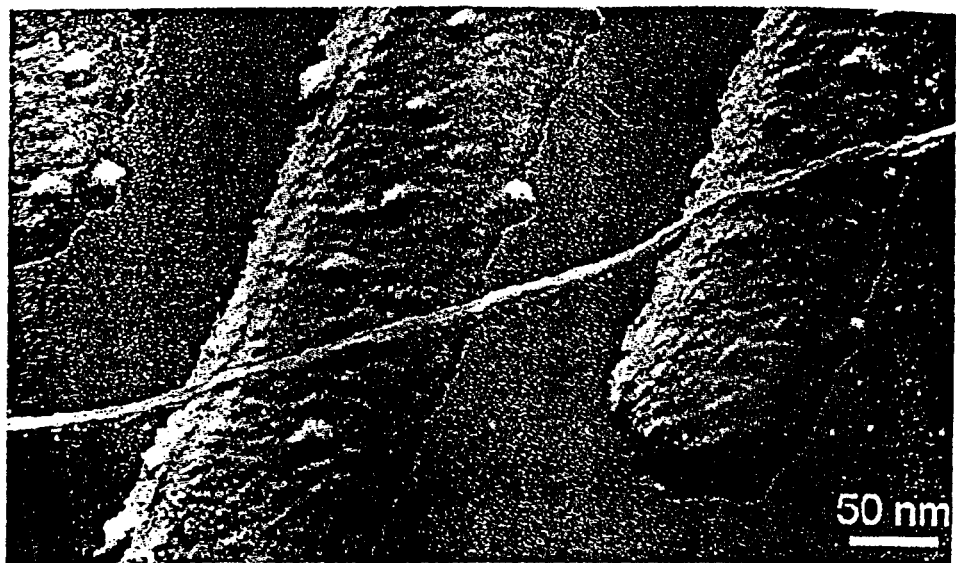


FIG. 1. Circuit fabrication using AFM manipulation. The scale is the same for each figure. (a) We begin with one vertical tube (main tube) and one horizontal tube (lasso tube). (b) A tube is brought in close proximity to main tube. (c) The tube is pushed against (perhaps on top of) the main tube. (d) Additional tubes are manipulated on top of the main tube. A piece of nanotube was broken off and sits near the lasso tube. (e) The lasso tube is opened and unwanted tubes pushed away. (f) AFM manipulation causes SWNT bundles to unravel.



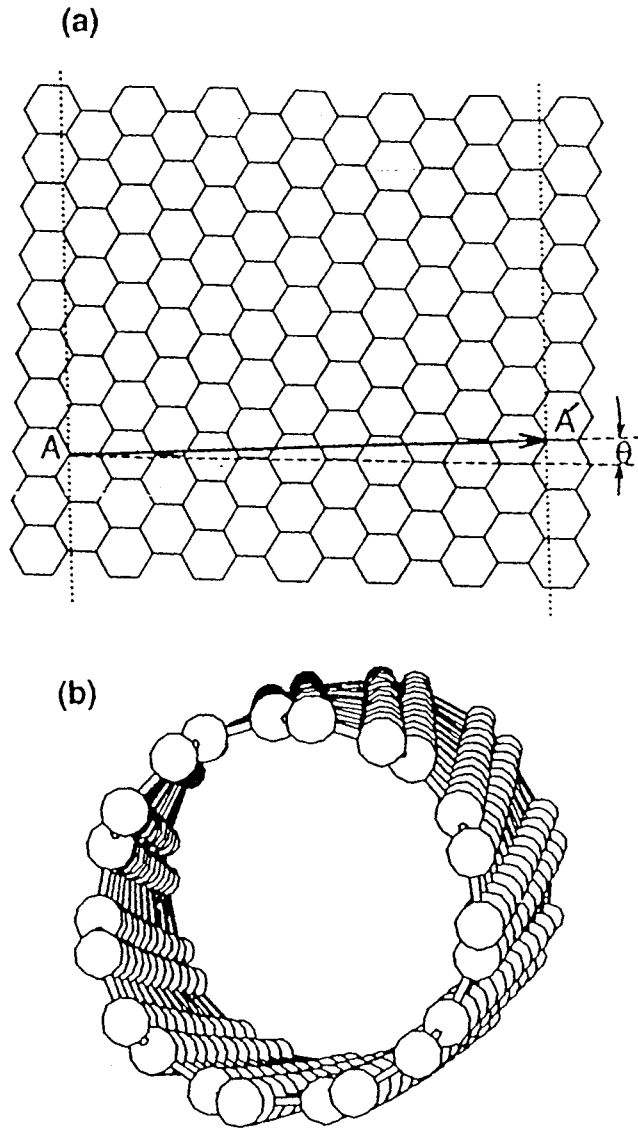
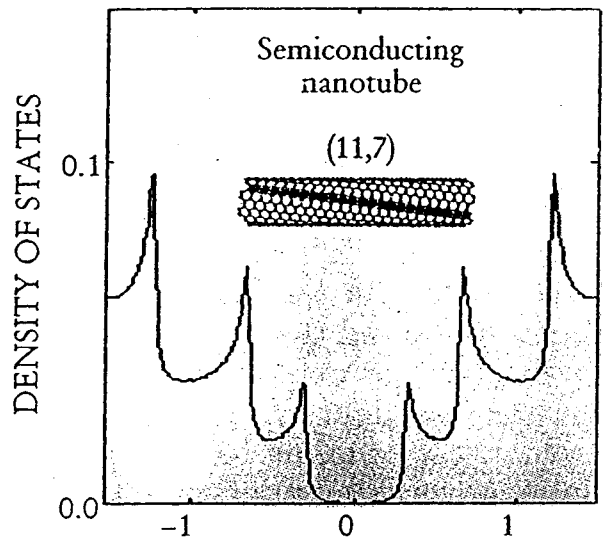
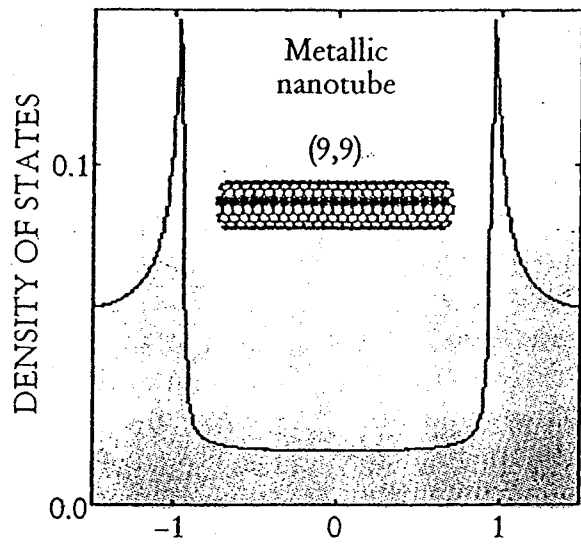
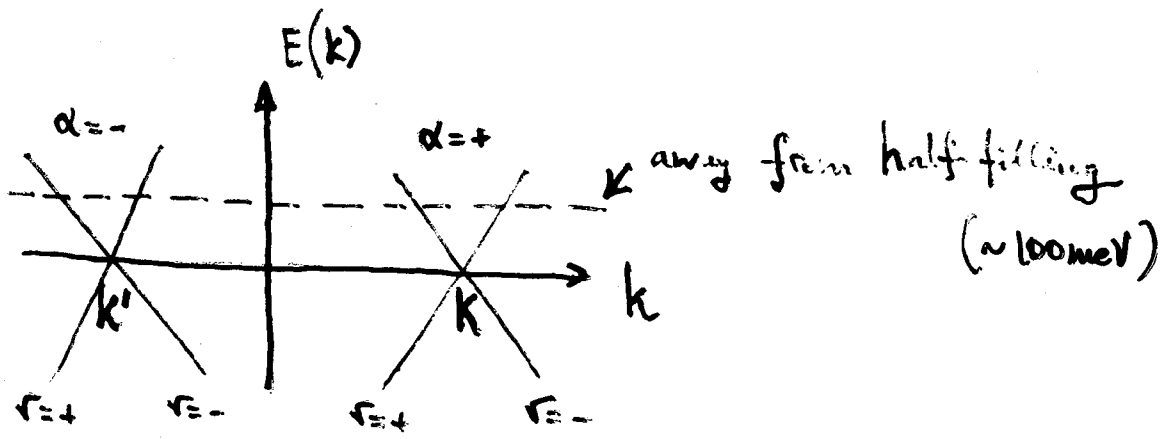


FIG. 3. (a) The vector $\vec{AA'}$ specifies a chiral fiber. We connect two dotted lines, normal to $\vec{AA'}$ at A and A' , to form a chiral fiber. (b) Atomic arrangement of the corresponding chiral fiber. The vector specifying an armchair has $\theta = 0^\circ$ and a zigzag fiber has $\theta = 30^\circ$.





$$\Psi_{\sigma}(\vec{r}) = \sum_{\alpha} \int_{\alpha} \Psi_{\alpha}(\vec{r}) \psi_{\alpha\sigma}(\vec{r})$$

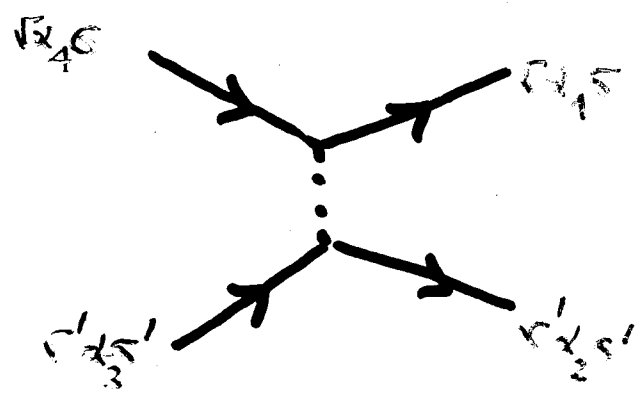
1D electron operators

$$H_0 = -i v \sum_{\alpha\sigma} \int dx \psi_{\alpha\sigma}^{\dagger} \partial_x \psi_{\alpha\sigma}$$

and

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

$$H_{\text{int}} = \frac{1}{2} \sum_{\sigma\sigma'} \sum_{\alpha_1 \dots \alpha_4} \int dx dx' V_{\alpha_1 \alpha_2 \alpha_3 \alpha_4}(\vec{r}-\vec{r}') \psi_{\alpha_1 \sigma}^{\dagger}(x) \psi_{\alpha_2 \sigma'}^{\dagger}(x') * \psi_{\alpha_3 \sigma'}(x') \psi_{\alpha_4 \sigma}(x)$$



Egger and G ('97, '98;
Kane, Balents,
MPA Fisher ('97)

Most important: forward scattering

$$H_{FS}^{(b)} = \frac{1}{2} \int dx dx' \rho(x) V(x-x') \rho(x')$$

total 1D density

$$\rho = \sum_{\alpha\sigma} \psi_{\alpha\sigma}^{\dagger} \psi_{\alpha\sigma}$$

$$\hookrightarrow V(k) = \frac{2e^2}{\pi} \ln(1/kR)$$

(x ~ 1.5)

Other interactions are "irrelevant"

Bosonization: $\psi_{\alpha\sigma} \sim e^{i\varphi_{\alpha\sigma}(x)} e^{ik_{\alpha\sigma}x + i\varphi_{\alpha\sigma}(0)}$

$$\phi_{c+} = \frac{1}{2} \sum_{\alpha\sigma} \psi_{\alpha\sigma} \leftarrow \text{total charge}$$

$$\phi_{c-} = \frac{1}{2} \sum_{\alpha\sigma} \alpha \psi_{\alpha\sigma} \leftarrow \text{charge flavour}$$

$$\phi_{s+} = \frac{1}{2} \sum_{\alpha\sigma} \sigma \psi_{\alpha\sigma} \leftarrow \text{total spin}$$

$$\phi_{s-} = \frac{1}{2} \sum_{\alpha\sigma} \alpha \sigma \psi_{\alpha\sigma} \leftarrow \text{spin flavour}$$

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

The LL tube Hamiltonian:

$$H = \frac{1}{2} \sum_{j=c^{\pm}, s^{\pm}} u_j \int dx \left[K_j \Pi_j^2 + \frac{1}{K_j} (\partial \phi_j)^2 \right]; \quad u_j = v/K_j$$

$$K_{c^{\pm}} = K_{s^{\pm}} = 1; \quad K_{c^+} = K = \left[1 + \frac{8e^2}{\pi v \alpha} \ln\left(\frac{L}{R}\right) \right]^{-1/2}$$

the LL parameter for a nanotube

Nanotube = (renormalised plasmon) +
+ (3 free bosons)

$$\text{Charging energy: } E_c = \frac{1}{2L^2} \int dx dx' \frac{e^2}{\alpha |x-x'|} \approx \frac{e^2}{\alpha L} \ln\left(\frac{L}{R}\right)$$

For Tans, et al (Nature '97), $E_c = 2.6 \text{ mV}$, $L = 3 \mu\text{m} \rightarrow K \approx 0.2$

Bockrath, et al (Nature '99), several devices $\rightarrow K \approx 0.28$

From bosonization formulas for $\psi \sim e^{i\varphi}$, follows that:

Theory ($K=0.28$)		Experiment (Bockrath, et al '99)
$\alpha_{\text{bulk}} = \frac{1}{8} \left(K + \frac{1}{K} - 2 \right)$	0.24	0.3 ($\div 0.05$)
$\alpha_{\text{edge}} = \frac{1}{4} \left(\frac{1}{K} - 1 \right)$	0.65	0.6

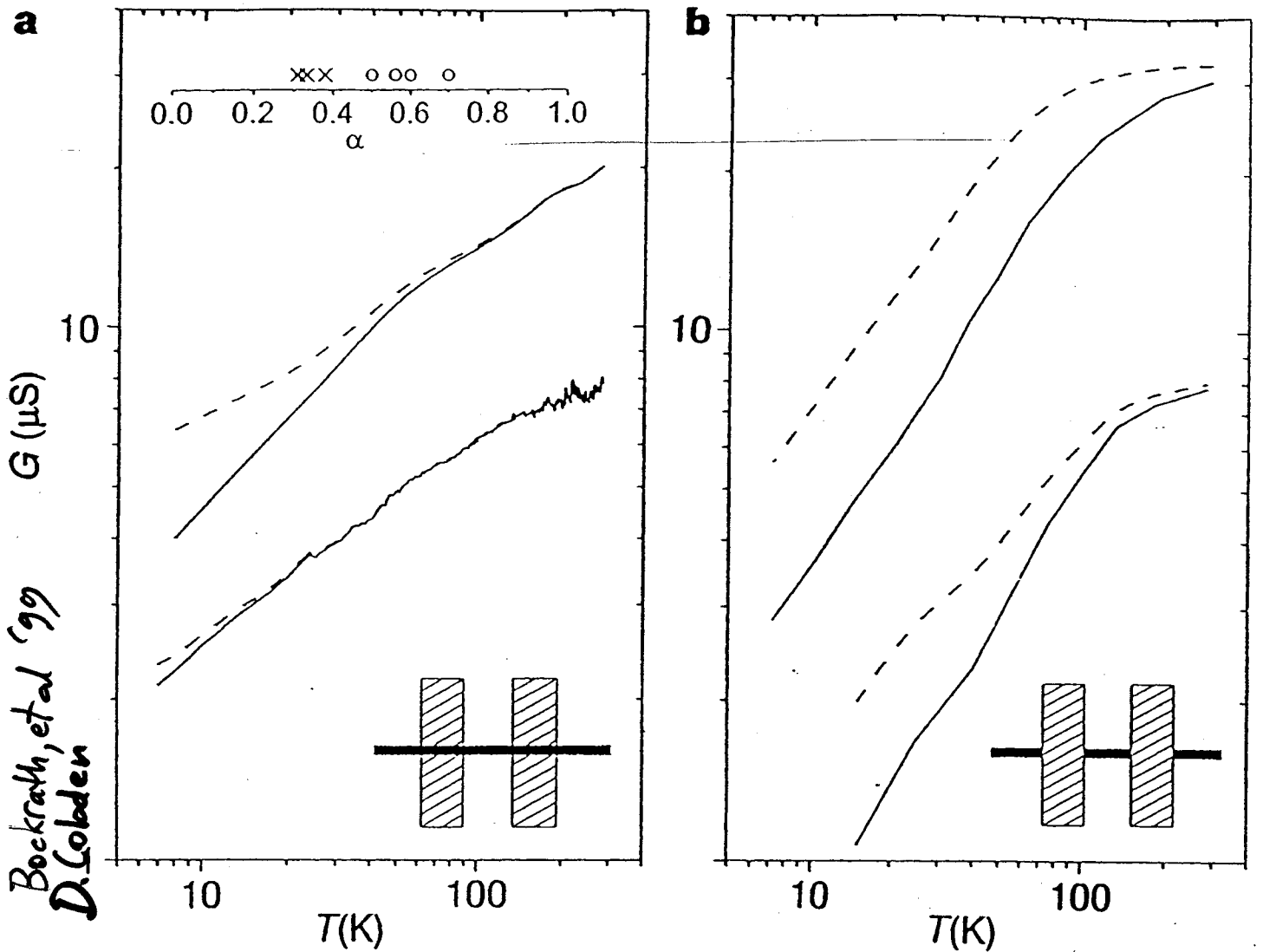


Figure 2 Conductance G plotted against temperature T for individual nanotube ropes. The data are plotted on a log-log scale. **a**, Data for ropes that are deposited over pre-defined leads (bulk-contacted); **b**, data for ropes that are contacted by evaporating the leads on top of the ropes (end-contacted). Sketches depicting the measurement configuration are shown in the lower insets. The plots show both the raw data (solid line) and the data corrected for the temperature dependence expected from the Coulomb blockade (CB) model (dashed line). We correct the data by dividing the measured $G(T)$ by the theoretically expected temperature dependence in the CB model. This correction factor depends only on $U/k_B T$, and, because U can be independently measured from the temperature dependence of the Coulomb oscillations, the correction procedure requires no adjustable

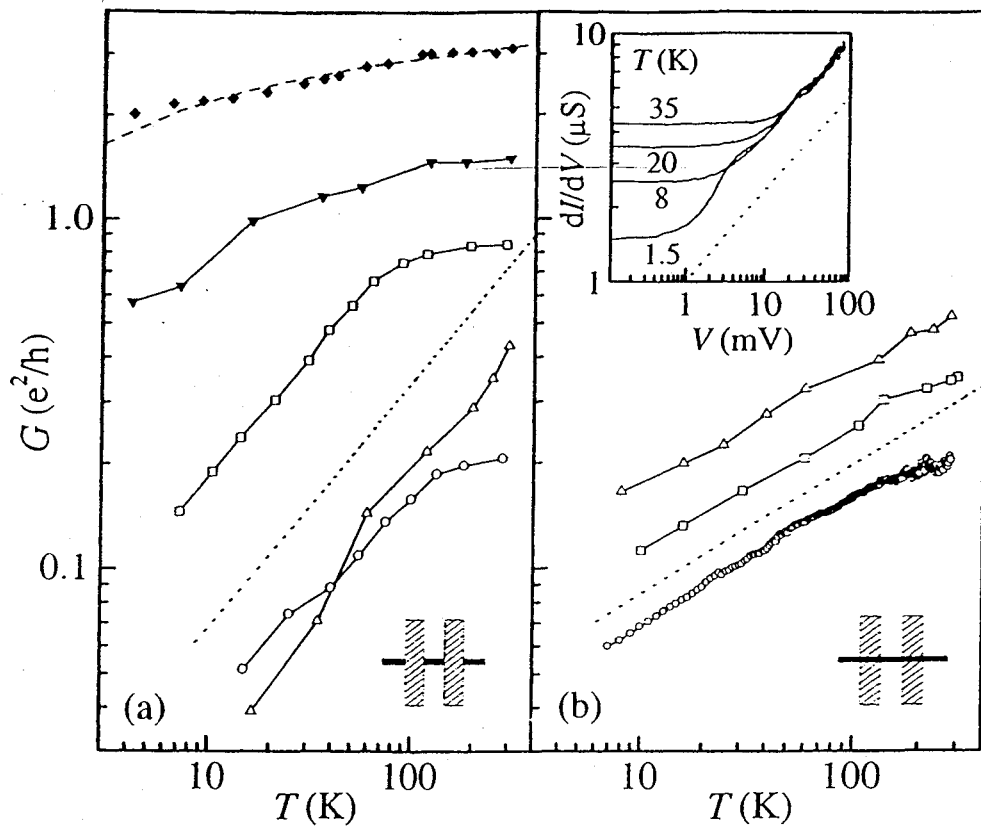


Fig. 7a,b. Conductance (averaged over V_g) vs. temperature for several devices. The data plotted with *open symbols* have been corrected for Coulomb blockade, whereas the others have not. **a** Metal-on-tube devices. The *open circles* correspond to the data in Fig. 3. The *dotted line* indicates $G \propto T^{0.7}$. The *dashed line* is a fit to $G = G_0 - aT^b$ with $G_0 = 4$, giving $b = -0.22$. **b** Tube-on-metal devices. The *dotted line* here indicates $G \propto T^{0.37}$. *Inset*: dI/dV vs. V at several temperatures for a tube-on-metal device. The *dotted line* here indicates $dI/dV \propto V^{0.37}$.

Nygaard, et al '99

Bockrath et al '99

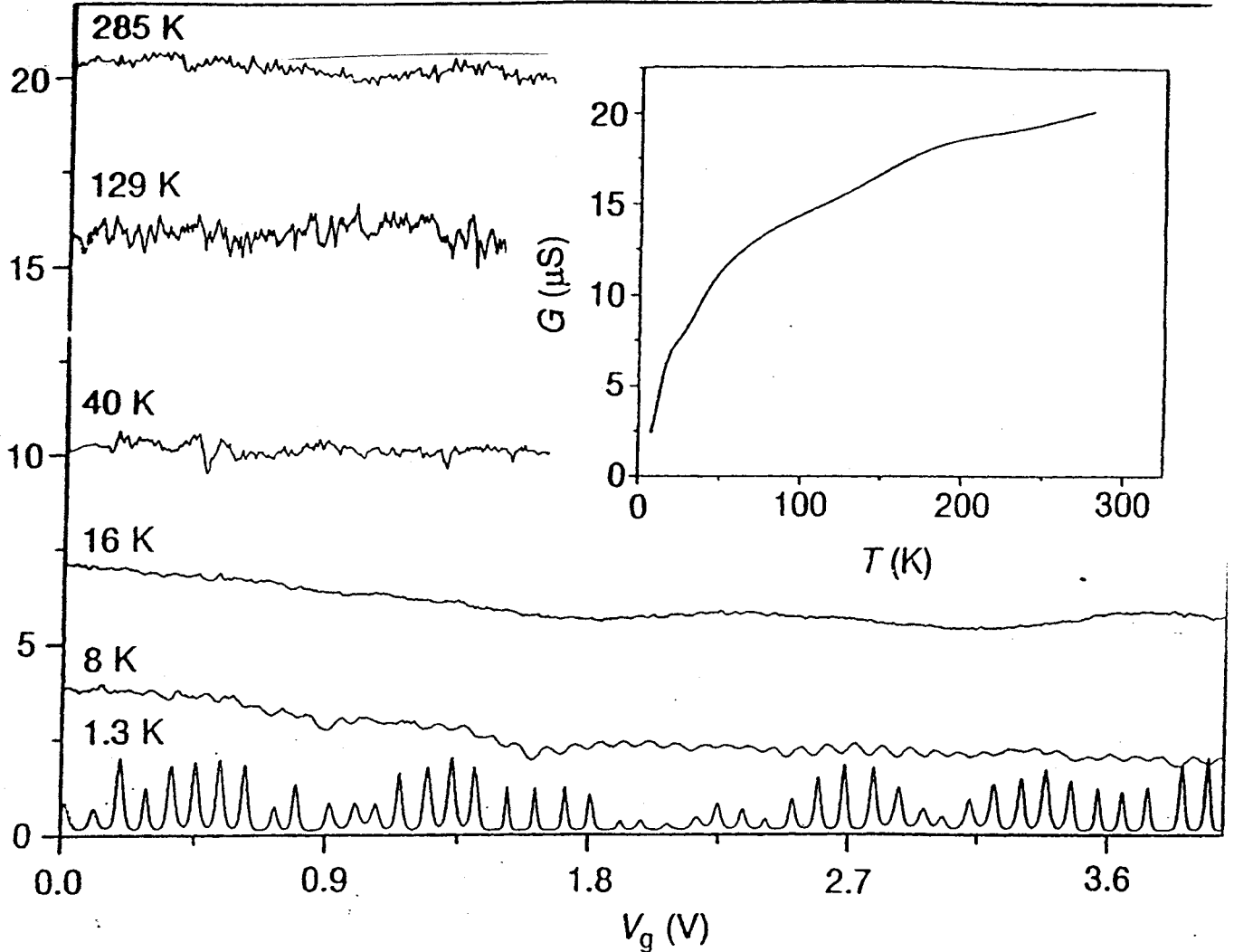


Figure 1 The two-terminal linear-response conductance G versus gate voltage V_g for a bulk-contacted metallic nanotube rope at a variety of temperatures. The data show significant temperature dependence for energy scales above the charging energy that cannot be explained by the Coulomb blockade model. Inset: average conductance as a function of temperature T . The samples used in these experiments are made in one of two ways. In both methods, SWNTs are deposited from a suspension in dichloroethane onto a 1- μm -thick layer of SiO_2 that has been thermally grown on a degenerately doped Si wafer, used as a gate electrode. Atomic force microscopy imaging reveals that the diameters of the ropes vary between 1 and 10 nm. In the first method⁹, chromium-gold contacts are applied over the top of the nanotube rope using electron beam lithography and lift-off. From measurements of these devices in the Coulomb blockade regime, we conclude that the electrons are confined to the length of rope between the leads. This implies that the leads cut the nanotube into

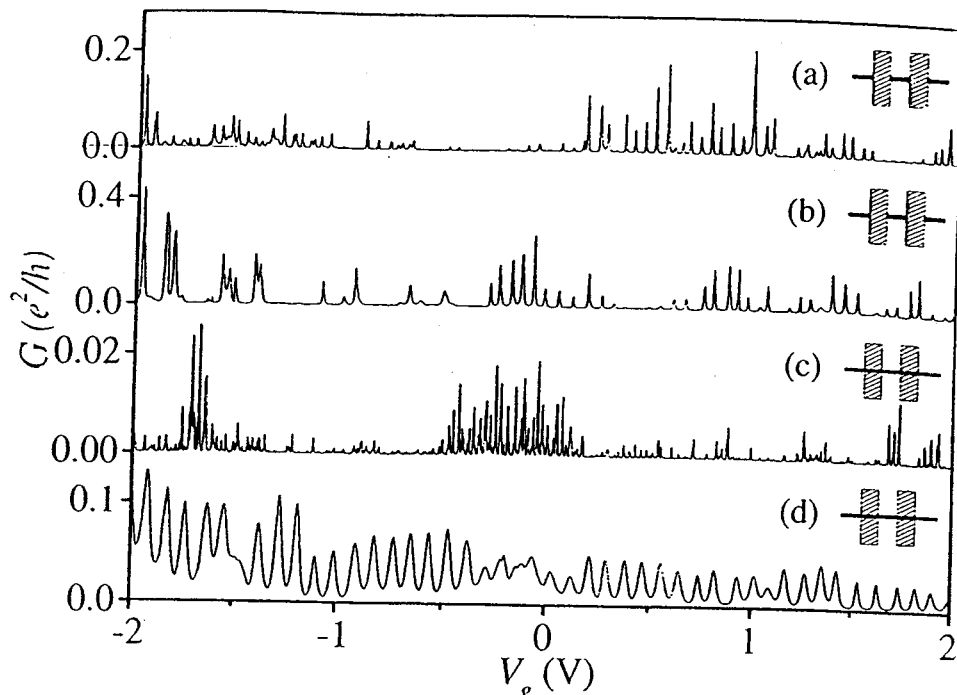


Fig. 4. $G - V_g$ for several devices at 4.2 K. As indicated by the insets, (a) and (b) are metal-on-tube, while (c) and (d) are tube-on-metal devices. Note that the oxide thickness is 350 nm for (a)–(c) and 1000 nm for (d)

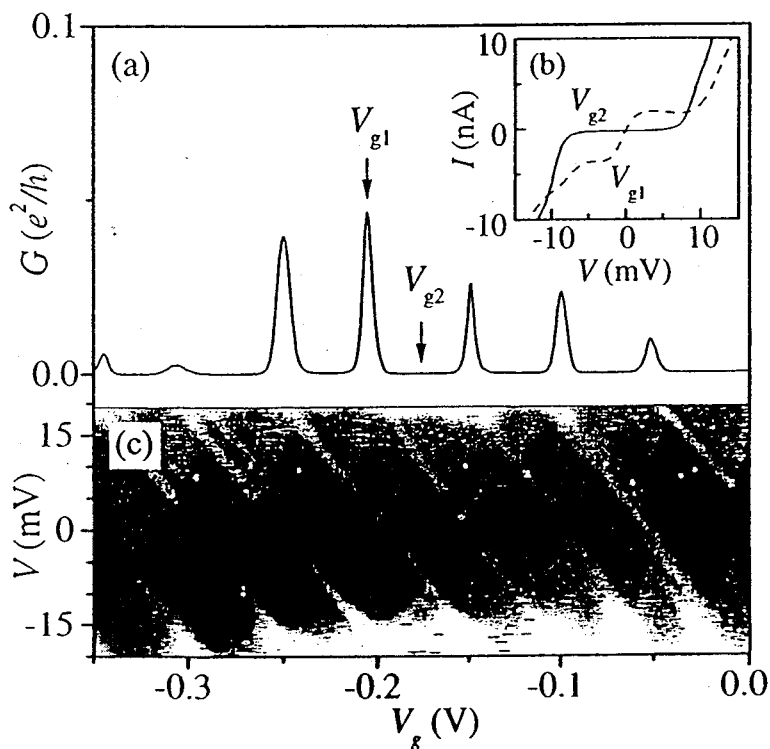


Fig. 5. a $G - V_g$ for a device at 4.2 K showing a regular series of CB peaks. b $I - V$ characteristics taken at the center of a peak (V_{g1}) and in between peaks (V_{g2}). c Grey scale (bias spectroscopy) plot of dI/dV vs. V_g and V at 4.2 K in the same range of V_g (lighter = more positive)

more between device to charging the full that the electron state over the contacts.

Figure 6 shows structure further, to 100 nm metal-on-tube device corresponding to the peaks are now sharp by device noise rather spectroscopy plot of R . The lines correspond very sharp.

A magnetic field is expected to modify Bohm type phase [30] indeed recently been reported tubes in this geometry ever too small for tubes where the flux linking a radius $r = 7 \text{ \AA}$

Nygaard, et al, '99

Scaling

For a weak link tunnelling conductance

$$G(V, T) = AT^\alpha \cosh\left(\frac{eV}{2k_B T}\right) \left| \Gamma\left(\frac{1+\alpha}{2} + \frac{ieV}{2\pi k_B T}\right) \right|^2$$

V - voltage drop across the link
 T - temperature

Scaling function

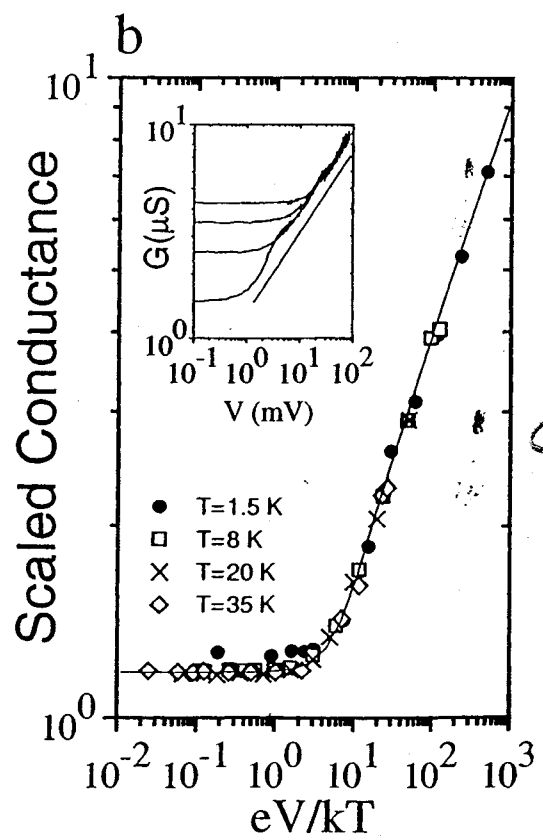
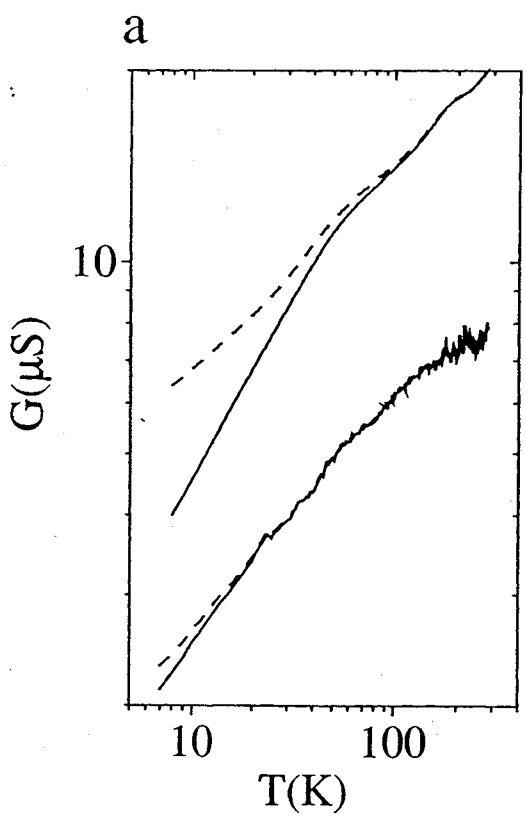


Fig. 7. (a) Conductance plotted against temperature on a double-logarithmic scale

from

Bockrath et al. Nature (1999)

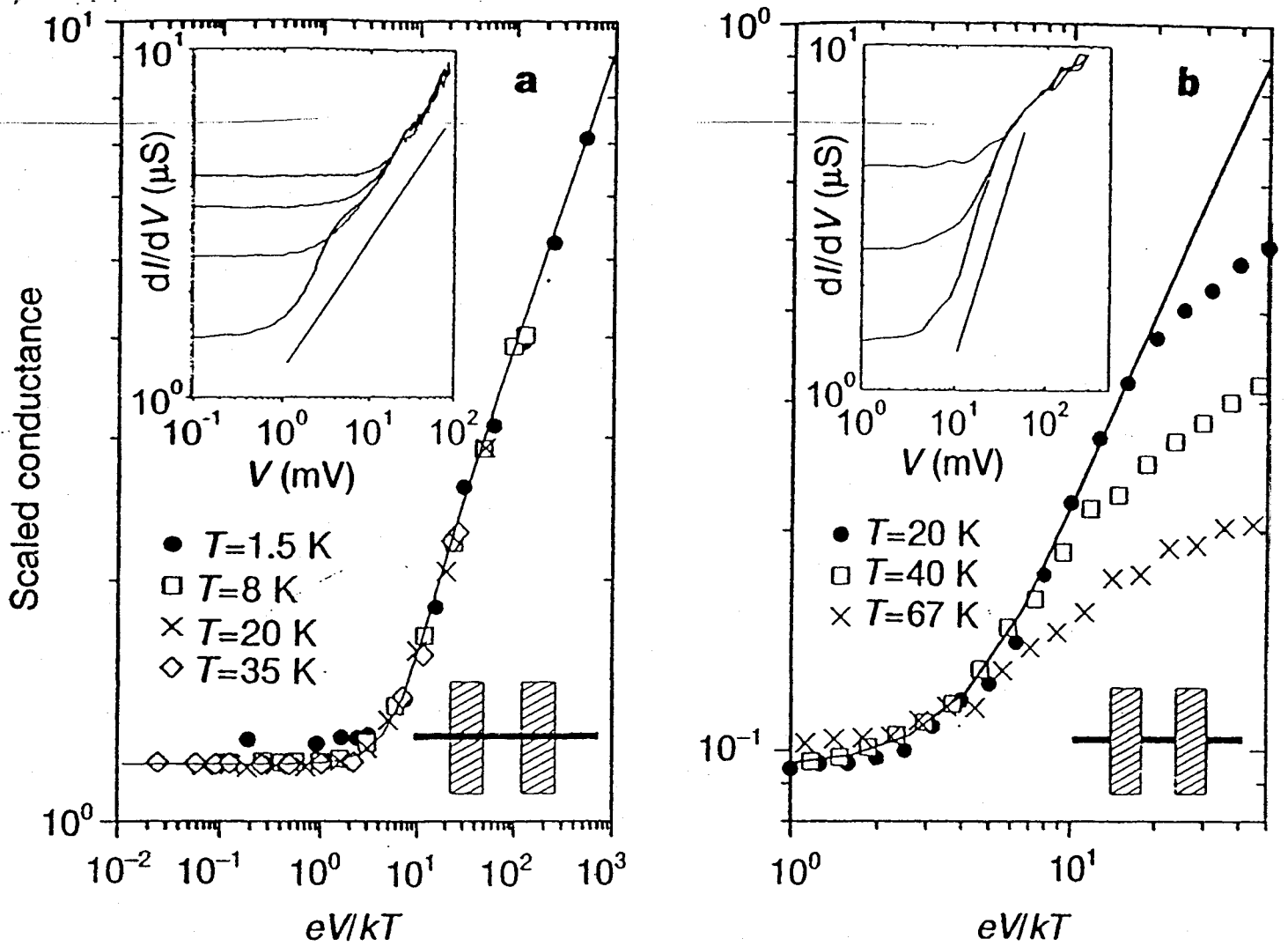
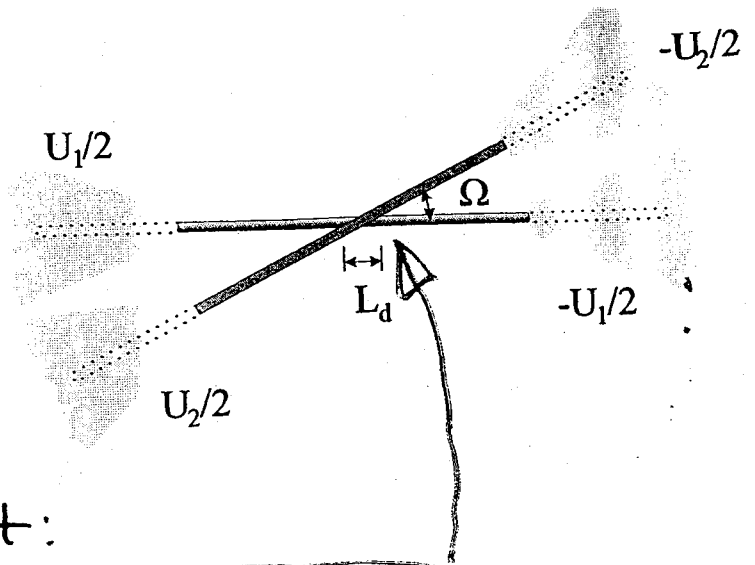


Figure 3 The differential conductance dI/dV measured at various temperatures. Inset in **a**, dI/dV curves taken on a bulk-contacted rope at temperatures $T = 1.6$ K, 8 K, 20 K and 35 K. Inset in **b**, dI/dV curves taken on an end-contacted rope at temperatures $T = 20$ K, 40 K and 67 K. In both insets, a straight line on the log-log plot is shown as a guide to the eye to indicate power-law behaviour. The main panels **a** and **b** show these measurements collapsed onto a single curve by using the scaling relations described in the text. The solid line is the theoretical result fitted to the data by using γ as a fitting parameter. The values of γ resulting in the best fit to the data are $\gamma = 0.46$ in **a** and $\gamma = 0.63$ in **b**.

Crossed set-up

(Komnik & Egger PRL (1998))



The only important interaction at the contact:

$$H_{\text{int}} = \lambda \cos[\sqrt{4\pi g} \Phi_1(0)] \cos[\sqrt{4\pi g} \Phi_2(0)]$$

In the relative channels, $\Phi_{\pm} = \frac{1}{\sqrt{2}} [\Phi_1 \pm \Phi_2]$, this decouples into two sine-Gordon models:

$$H_{\pm} = H_0[\phi_{\pm}] \pm (\lambda/2) \cos[\sqrt{8\pi g} \Phi_{\pm}(0)] \leftarrow \text{solvable}$$

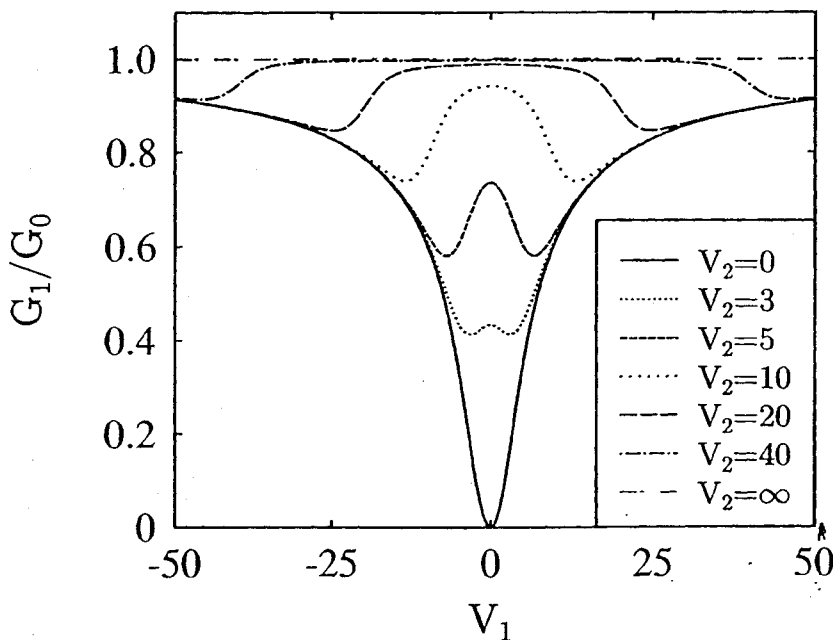
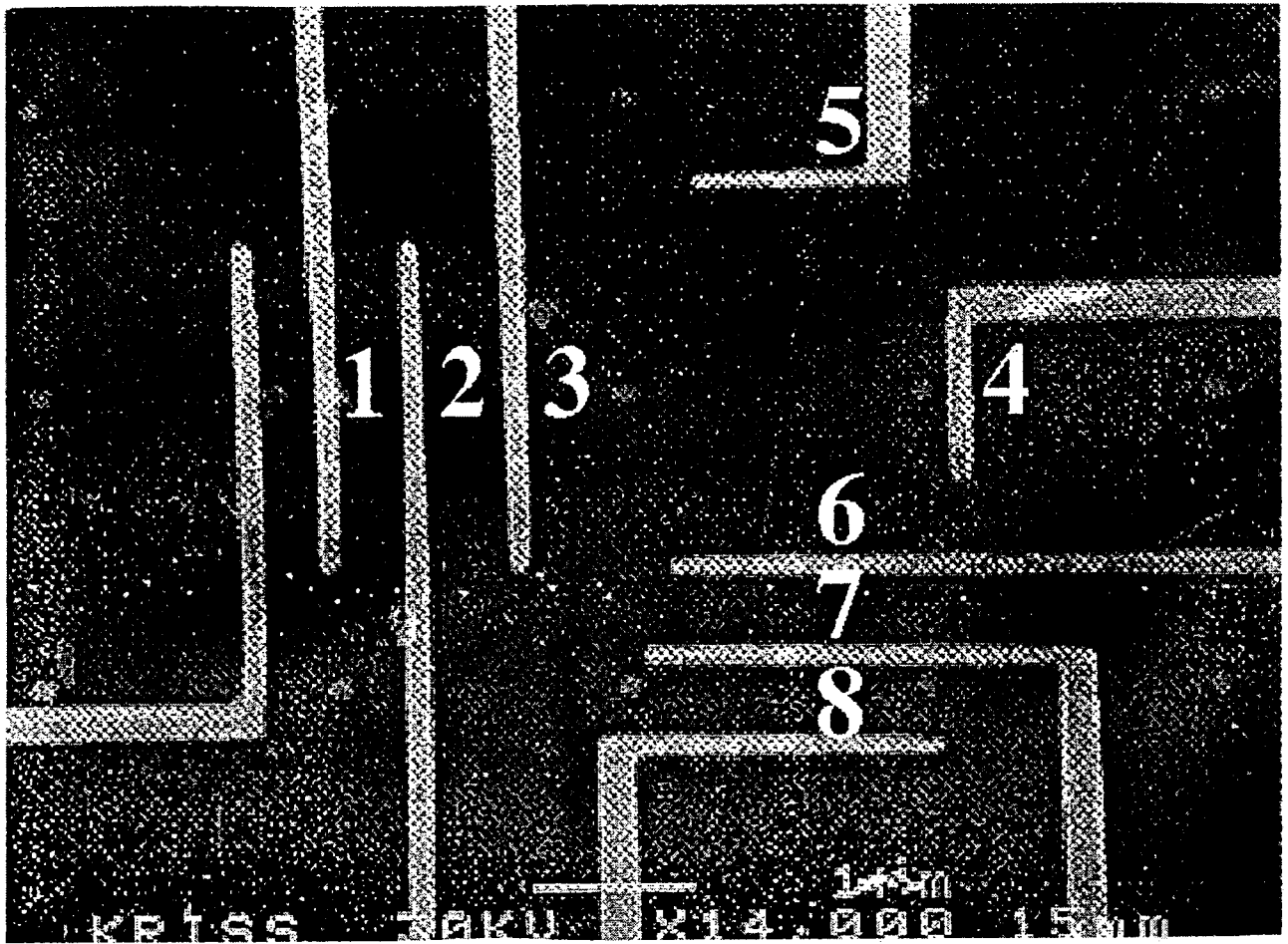
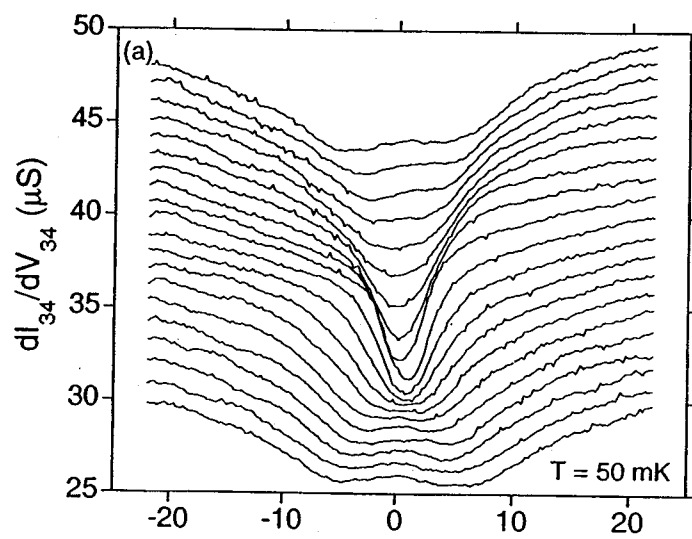


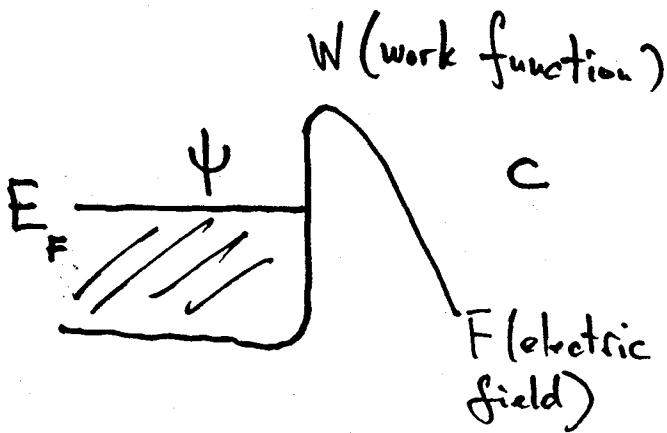
Fig. 3. Conductance $G_1/G_0 \equiv I_1/(e^2 V_1/h)$ for $g = 1/4$, $T = 0$, and several values of the cross voltage V_2 . The overall energy scale is set by the coupling λ .



From Kim et al. cond-mat/0005083.



Field emission



$$H = H_0[c] + H_{LL}[\psi] + \gamma [\psi^\dagger(0)c(0) + c^\dagger(0)\psi(0)]$$

tunnelling

Energy resolved current $\rightarrow J(\omega) = \mathcal{F} \mathcal{D}(\omega) n(\omega)$

\mathcal{F} is the form factor of the emitter, $n(\omega)$ is the energy distribution function of the electrons in the emitter and $\mathcal{D}(\omega)$ is the transmission coefficient of the barrier. For the triangularly-shaped one

$$\mathcal{D}(\omega) \sim \exp(-4\sqrt{2m}(W - \omega)^{3/2}/3\hbar F)$$

At lowest order in γ : $n(\omega)$ - equilibrium distribution

In the case of Luttinger liquids:

$$n(\omega) = \Theta(E_F - \omega) |\omega - E_F|^{1/g-1} / a_0 D^{1/g} \Gamma(1/g)$$

\Rightarrow

- $J(\omega)$ has exponential behaviour below E_F
- $J(\omega) \sim |\omega - E_F|^{1/g-1}$ in immediate vicinity of E_F
- generalisation of Fowler-Nordheim law to LLs:

sharp edge!

$$J = \frac{\mathcal{F}}{a_0 D^{1/g}} \left[\frac{F^2}{4k_F W} \right]^{1/2g} \exp\left(-\frac{4k_F^{1/2}}{3F} W^{3/2}\right)$$

- $J(\omega) = 0$ above E_F

\Rightarrow this is in fact not true, hence interactions and higher orders in γ needed

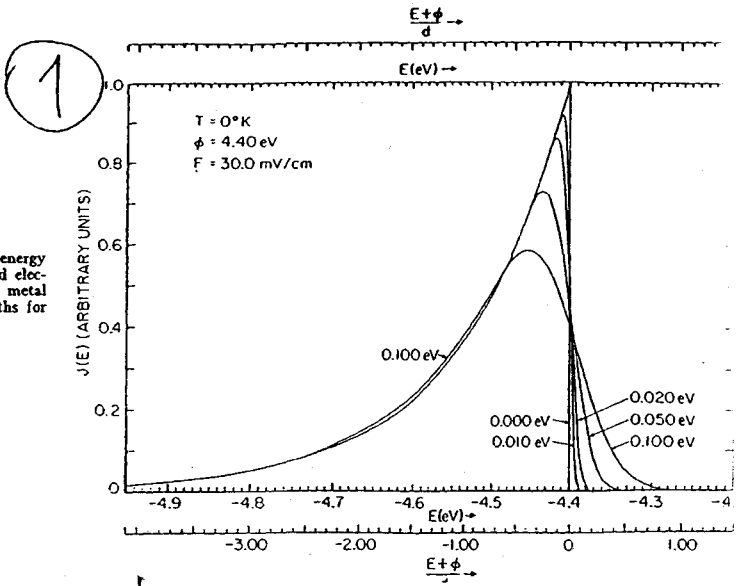


FIG. 7. Theoretical total energy distribution of field emitted electrons from a free-electron metal with various analyzer widths for zero temperature. (YK68.)

3

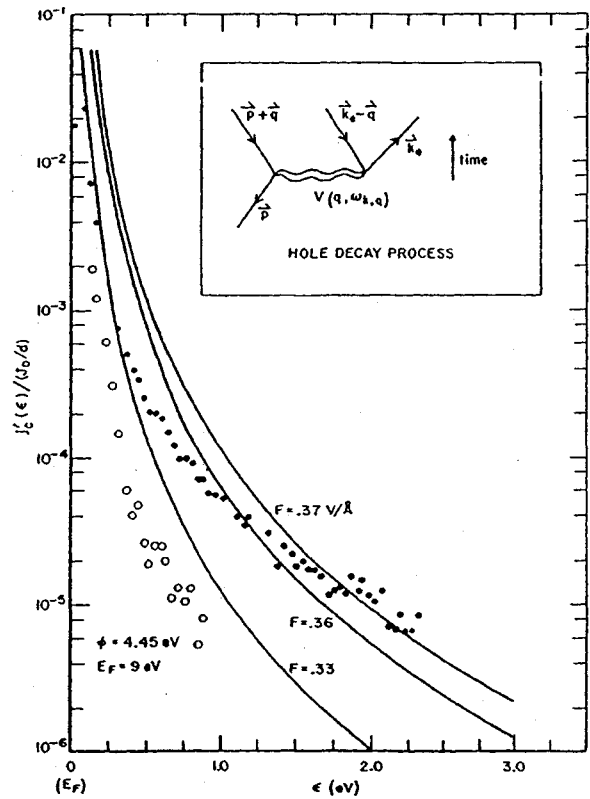


FIG. 2. Solid lines: theoretical calculations for the high-energy tail of the TED for fields 0.33, 0.36, and 0.37 V/Å. These curves rise to $dj/dε=1$ at $ε=0$, and then decay exponentially for $ε < 0$ in the well understood way shown in Fig. 1. Closed circles: experimental points for $F=0.37$ V/Å; open circles: for 0.326 V/Å. Inset: Diagram illustrating the hole-damping mechanism in which a hole of energy-momentum E_p, \vec{p} scatters from the electron gas exciting an electron-hole pair of energy-momentum ω_{eh}, \vec{p} . The electron momentum is \vec{k}_e .

'Secondary current'

2

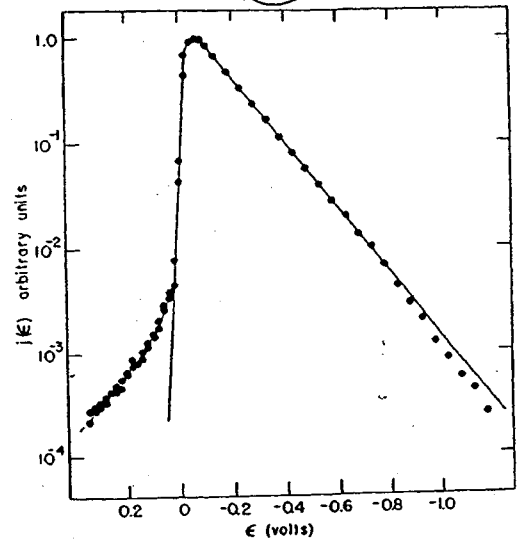
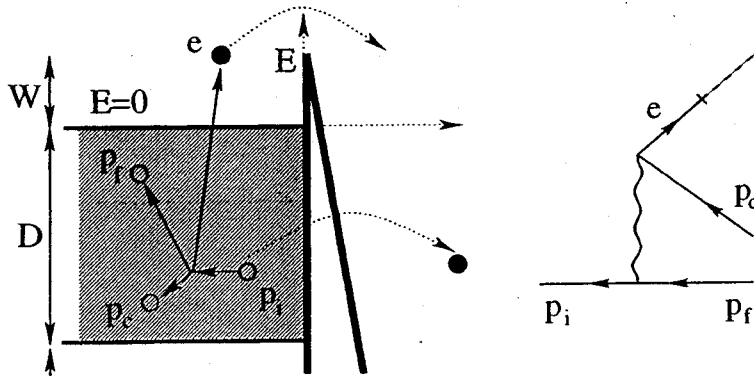


FIG. 2. Total energy distribution from the (120) plane at 20°K, with $F=0.300$ V/Å and a probe current after multiplication of 1×10^{-8} A. The points are experimental; the line, a convolution of Eq. (1) and a Gaussian analyzer transmission function with a full width at half-maximum of 40 meV.

From Lea & Gomer, PRL (1970)

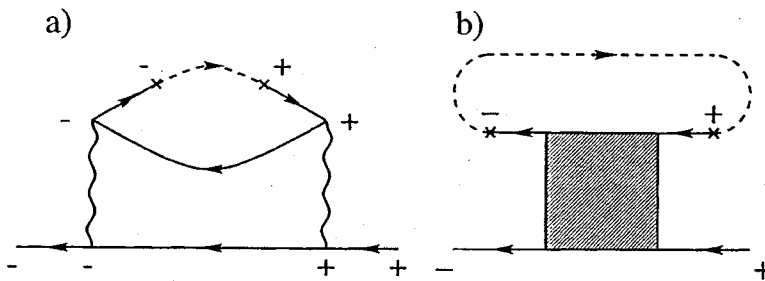
Qualitative explanation for secondary current:



Must calculate GF at the emitter's tip:

$$\delta g^{-+}(t_1, t_2) = \gamma^2 \int_C dt_3 dt_4 \mathcal{K}_C(t_1^-, t_2^+; t_3, t_4) G(t_3, t_4)$$

where $\mathcal{K}_C(t_1^-, t_2^+; t_3, t_4) = \langle T_C[\psi^\dagger(t_2^+) \psi^\dagger(t_3) \psi(t_4) \psi(t_1^-)] \rangle$ and $G(t_3, t_4)$ is the corresponding Green's function of c -operators



Spectral analysis:

$$j(\omega > E_F) \propto \lim_{V_b \rightarrow \infty} \int_{-\infty}^{\infty} dt \frac{e^{i(\omega - E_F - V_b)t}}{t + i\alpha} \int_0^{\infty} d\tau_1 \int_0^{\infty} d\tau_2 e^{i(\omega - E_F)(\tau_1 + \tau_2)} \times \langle \{ \psi^\dagger(\tau_1), \psi^\dagger(0) \} \{ \psi(t + \tau_1), \psi(t + \tau_1 + \tau_2) \} \rangle.$$

Brading

Luttinger braiding $\psi(t_1)\psi(t_2) = e^{i\pi \text{sign}(t_1 - t_2)/g} \psi(t_2)\psi(t_1)$, so

- $j(\omega > E_F) \sim \left(\frac{\omega - E_F}{D} \right)^\lambda$, where $\lambda = 1/g - 2$

- for single-wall carbon nanotubes substitute $1/g$ by $(1/K + 3)/4$, so

divergent / convergent threshold is $K_c = 1/5$

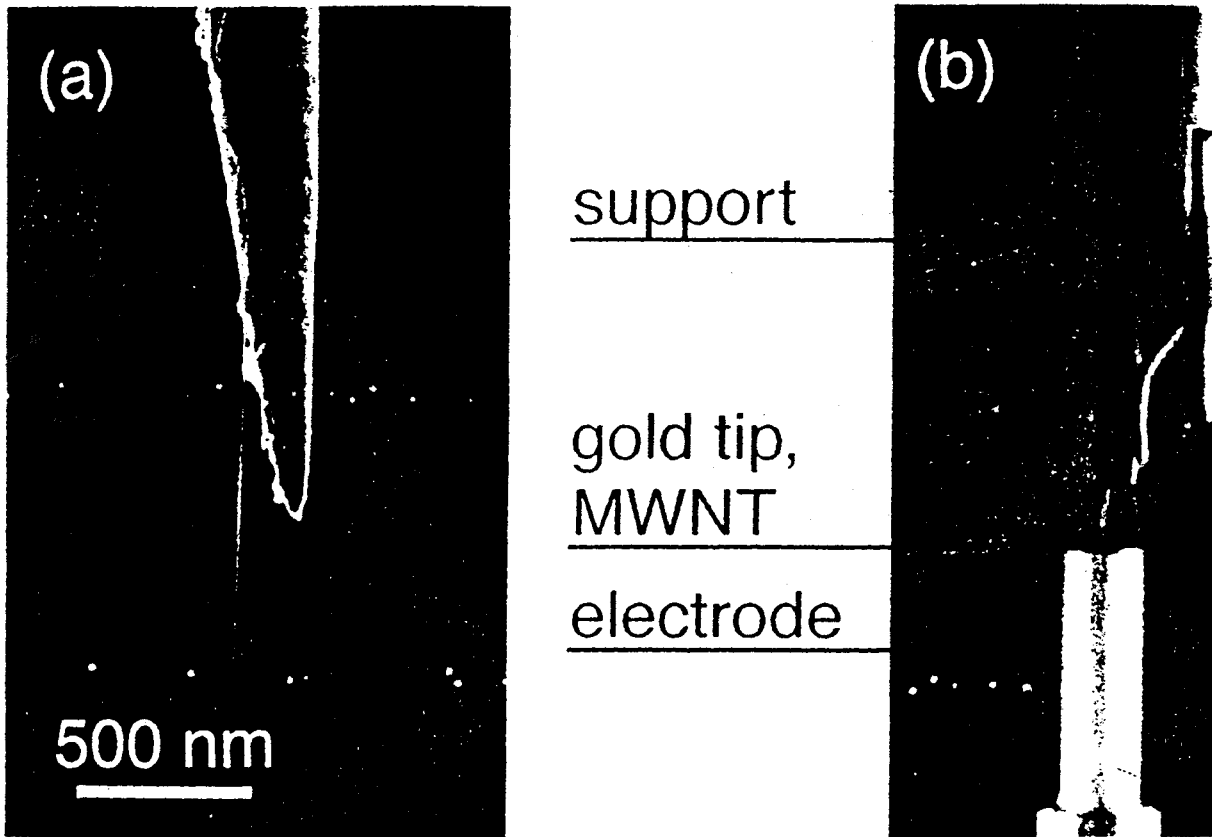


Fig. 2. a Single MWNT mounted on the tip of an etched gold wire. b Optical micrograph of the experimental setup for field emission: the wire is fixed on a support, and placed 1 mm above the cylindrical collector electrode.

From Bonard et al.
Appl. Phys (1999)