Carbon Nanostructures

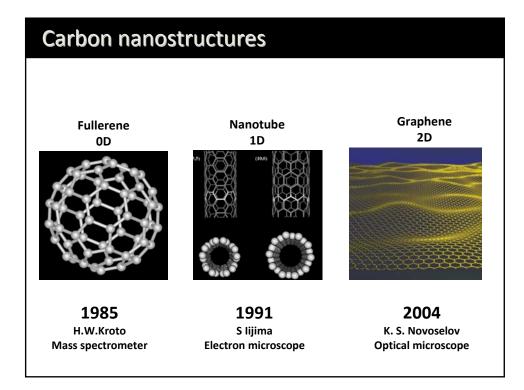
I. Graphene

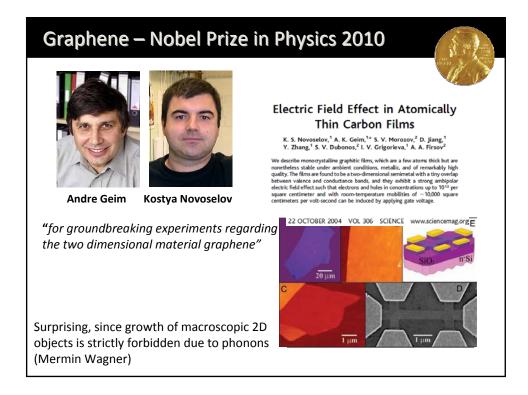
Outline:

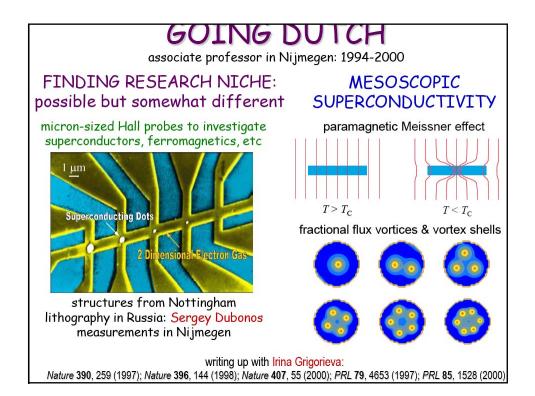
- Introduction (Making graphene, Applications, etc.)
- Band structure
- Physics of Dirac electrons (Barry phase, Klein tunneling)
- Half-Integer Quantum Hall Effect
- Mobility in Graphene

References:

- E. McCann Graphene monolayers Lancaster University, UK Tight-binding model, QHE
- C. Beenakker, Reviews of Modern Physics, 80, 1337 (2008)
- L. Tapaszto & J. Cserti talks, MAFIHE Teli Iskola a Grafenrol 2011, ELTE
- A. Geim talk, TNT Conference 2010 http://www.tntconf.org/2010/Presentaciones/TNT2010 Geim.pdf

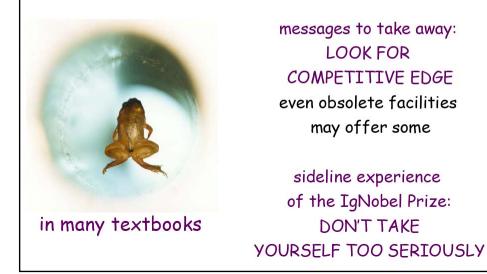




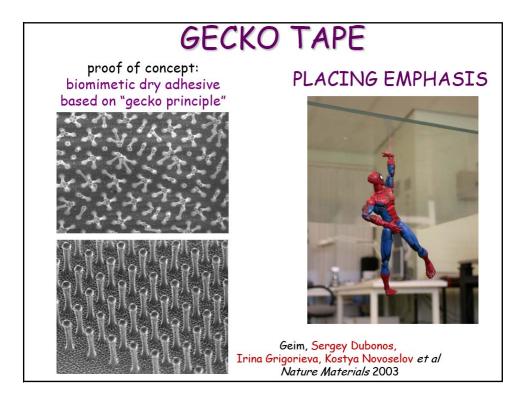


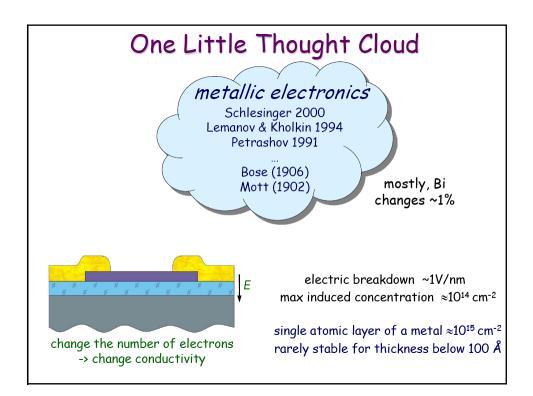
PERCEPTION CHANGE

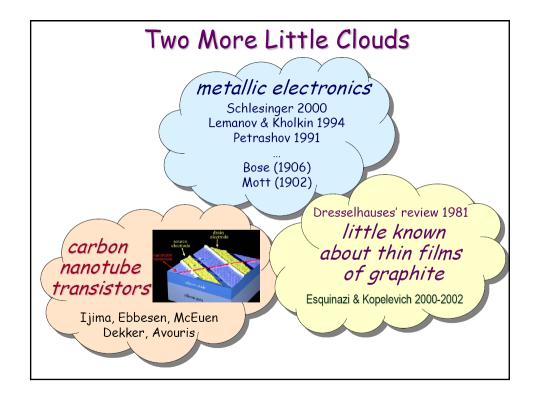
everything (and everybody) is magnetic; ever present diamagnetism is NOT negligible

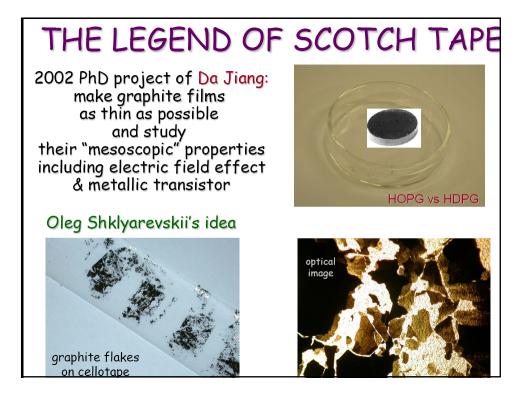


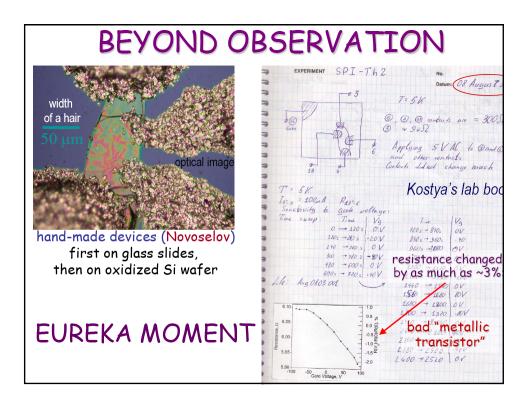


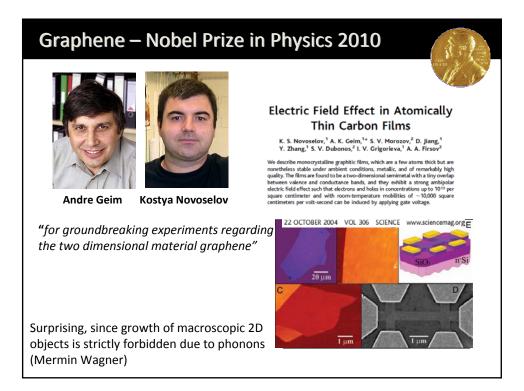


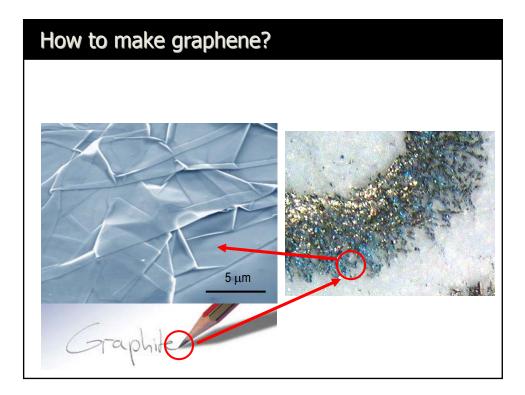


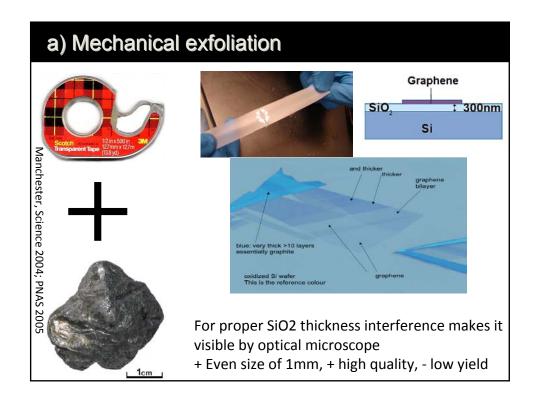


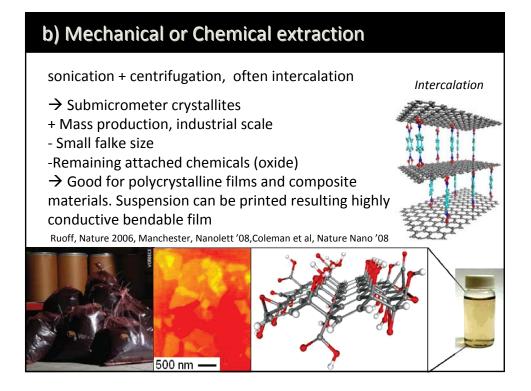












b) Epitaxial growth of a monolayer

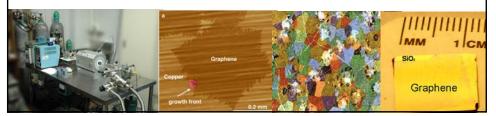
Grow a monolayer of C and chemically remove the substrate

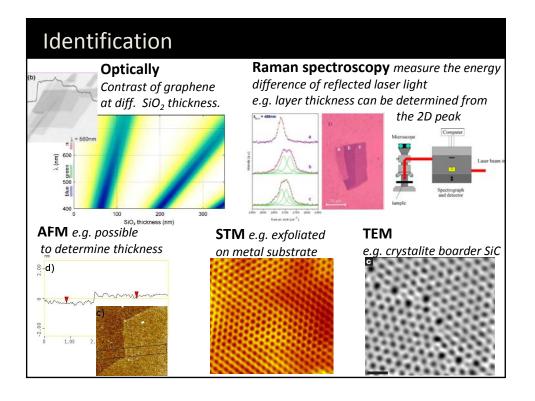
1)SiC substrate: (upper figs.)

SiC is insulator, Graphene layers grow as a carpet on the surface. Layers are electrically

well isolated (different stacking). Possible to grow 1,2 layers. - Difficult growth process

2) CVD on Cu, Ni (Lower figs.) "Easy" to do: T + gas flow. Self terminating process. Result: single layer, - polycrystalline, it follows the crystallites of the metal surface, Use HCl to remove substrate. (commercial available)



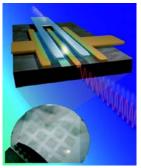


Properties, applications

Electronic properties:

- Truly 2D electron gas on the surface. New possibilities: SC, Ferro, high dielectrics, use local probes.
- Massless Dirac electrons

-Good electronic quality: submicrons without scattering @RT although adsorbates etc. Due to weak e-ph coupling mobility > 200000 cm²/Vs @ RT (Si: <1500 cm²/Vs) - Quantum effect at RT



transistor @ 300 GHz Nature 467, 305 (2010)

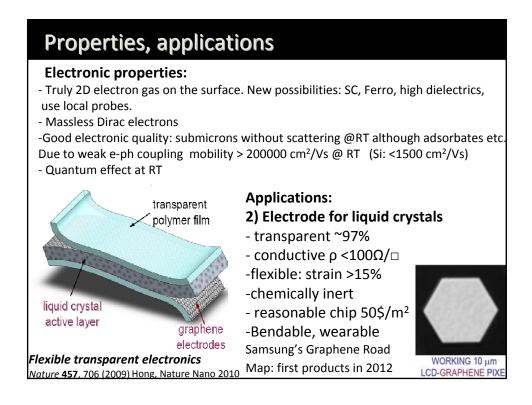
Applications:

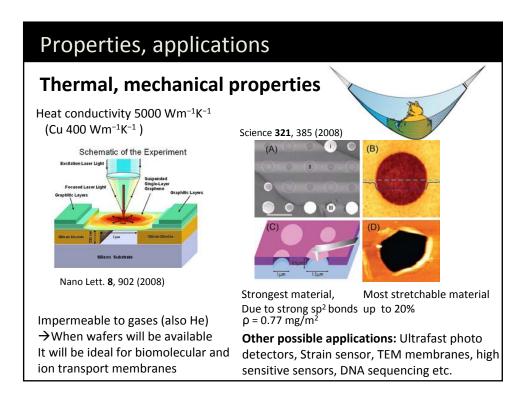
- 1) Ultra High Frequency Transistors
- Ballistic transport
- high velocity
- great electrostatics
- scales to nm size

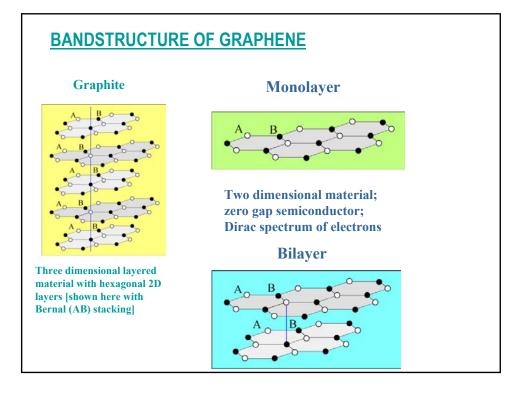
2009: 100 GHz (IBM & HRL)

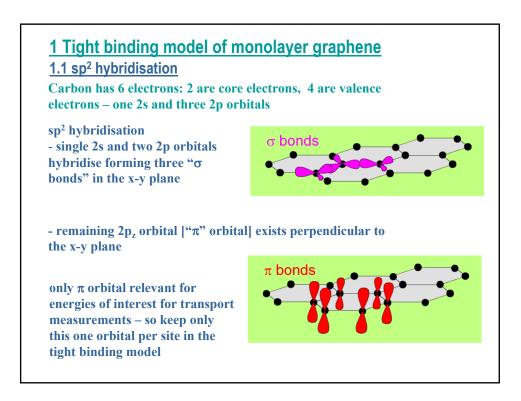
2010: 300 GHz (UCLA & Samsung)

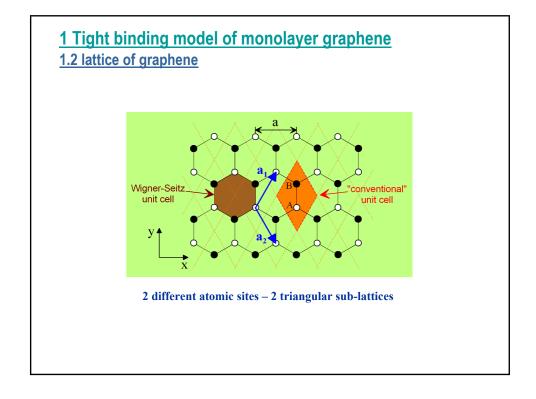
o GHz scaling >1THz

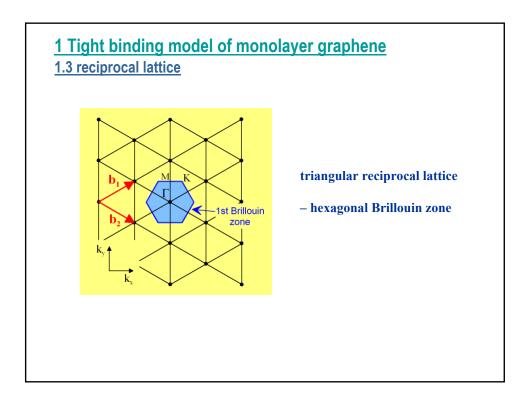


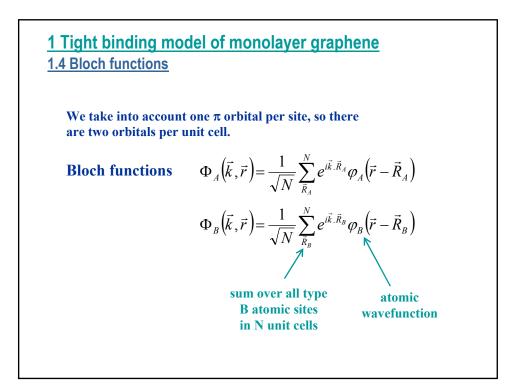


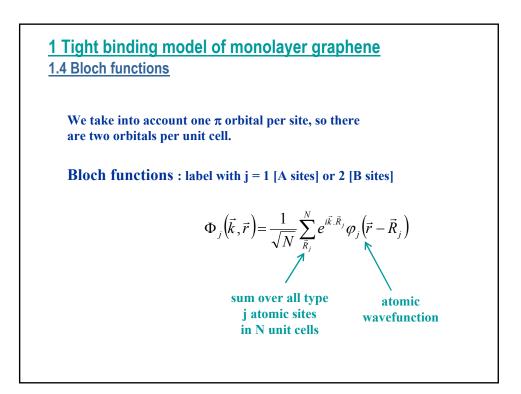


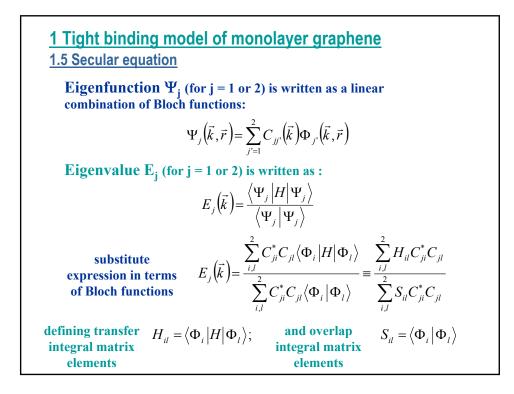












<u>1 Tight binding model of monolayer graphene</u> <u>1.5 Secular equation</u>

$$\sum_{l=1}^{2} H_{ml} C_{jl} = E_{j} \sum_{l=1}^{2} S_{ml} C_{jl}$$

Explicitly write out sums:

$$m = 1 \implies H_{11}C_{j1} + H_{12}C_{j2} = E_j (S_{11}C_{j1} + S_{12}C_{j2})$$

$$m = 2 \implies H_{21}C_{j1} + H_{22}C_{j2} = E_j (S_{21}C_{j1} + S_{22}C_{j2})$$

Write as a matrix equation:

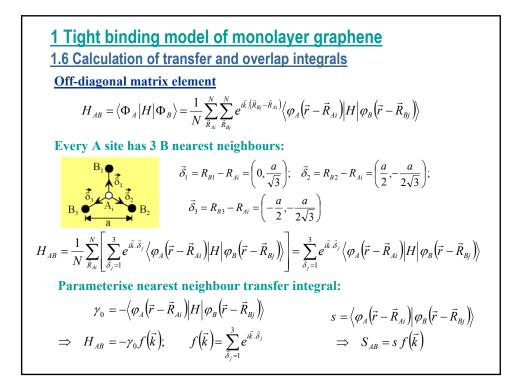
$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix} = E_j \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix}$$

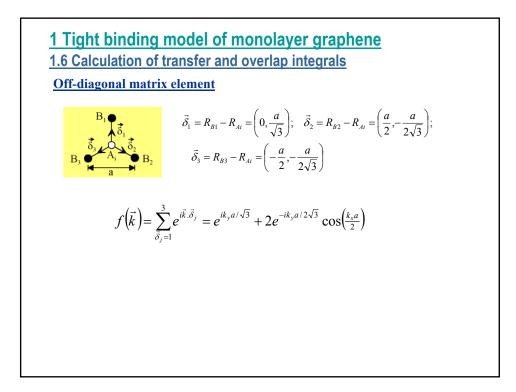
 $HC_i = E_i SC_i$

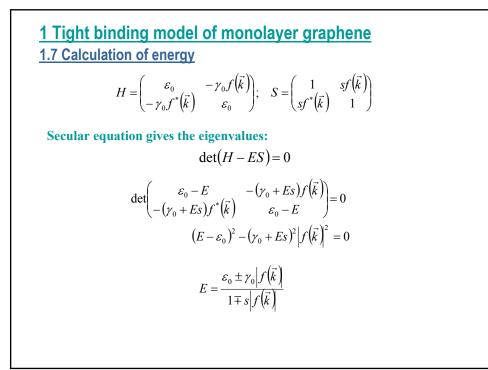
Secular equation gives the eigenvalues:

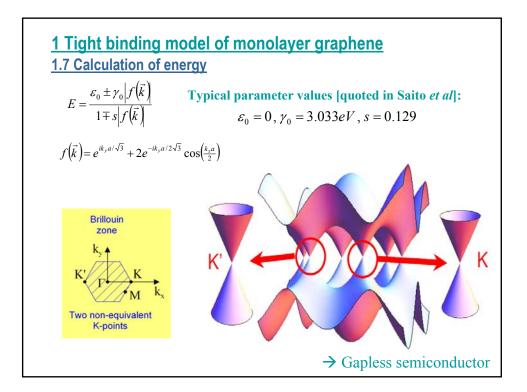
 $\det(H - ES) = 0$

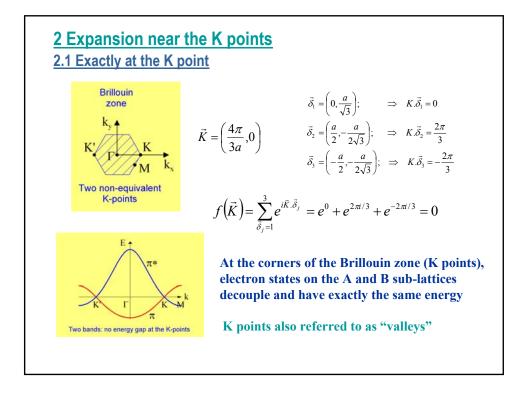
 $\frac{1 \text{ Tight binding model of monolayer graphene}}{1.6 \text{ Calculation of transfer and overlap integrals}} \\
H_{ij} = \langle \Phi_i | H | \Phi_j \rangle; \qquad S_{ij} = \langle \Phi_i | \Phi_j \rangle \qquad \Phi_j(\vec{k}, \vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}_j}^{N} e^{i\vec{k}.\vec{k}_j} \varphi_j(\vec{r} - \vec{k}_j) \\
\frac{\text{Diagonal matrix element}}{H_{AA}} = \langle \Phi_A | H | \Phi_A \rangle = \frac{1}{N} \sum_{\vec{k}_A}^{N} \sum_{\vec{k}_A}^{N} e^{i\vec{k}.(\vec{k}_A - \vec{k}_A)} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Aj}) \rangle \\
\frac{\text{Same site only:}}{H_{AA}} = \frac{1}{N} \sum_{\vec{k}_A}^{N} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \qquad S_{AA} = \frac{1}{N} \sum_{\vec{k}_A}^{N} \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \\
= \langle \varphi_A(\vec{r} - \vec{R}_{Ai}) | H | \varphi_A(\vec{r} - \vec{R}_{Ai}) \rangle \qquad = 1 \\
\text{A and B sites are chemically identical:} \\
H_{AA} = H_{BB} = \varepsilon_0 \qquad S_{AA} = S_{BB} = 1$

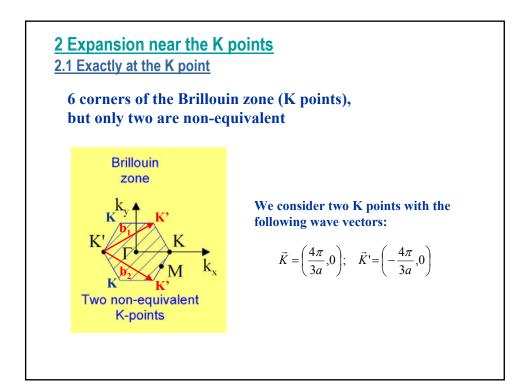


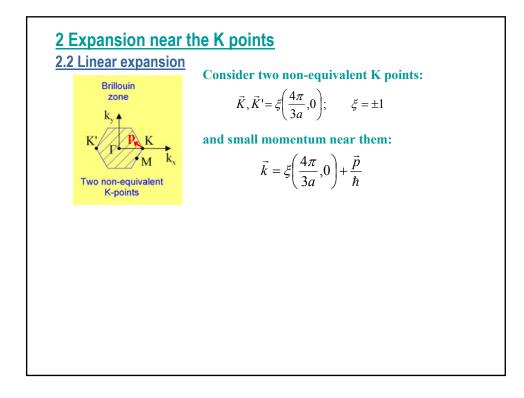


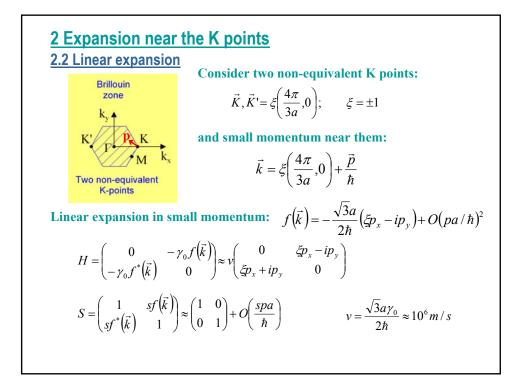










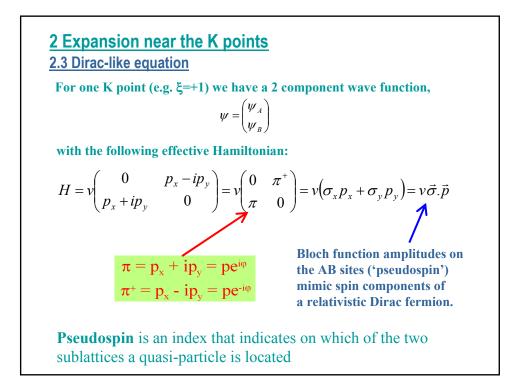


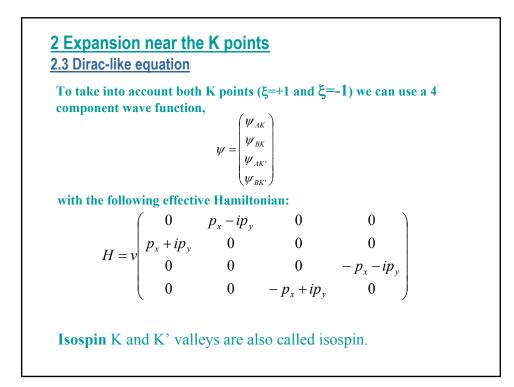
2 Expansion near the K points
3.2 Linear expansion

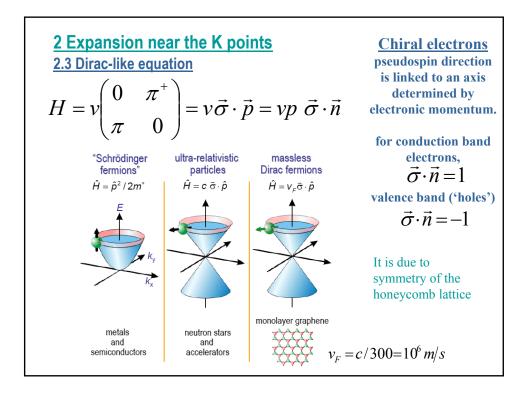
$$H = \begin{pmatrix} 0 \\ -\gamma_0 f^*(\vec{k}) \end{pmatrix} \stackrel{-\gamma_0 f(\vec{k})}{0} \approx v \begin{pmatrix} 0 \\ \xi p_x + i p_y \end{pmatrix} \stackrel{(\xi p_x - i p_y)}{0}$$

$$S = \begin{pmatrix} 1 \\ sf^*(\vec{k}) \end{pmatrix} \stackrel{sf(\vec{k})}{1} \approx \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + O \begin{pmatrix} spa \\ \hbar \end{pmatrix} \qquad v = \frac{\sqrt{3}a\gamma_0}{2\hbar} \approx 10^6 \, m/s$$
New notation for components on A and B sites
$$C_j = \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix} \Leftrightarrow \psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

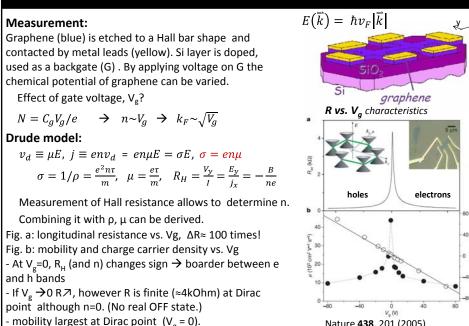
$$S^{-1}HC_j = E_jC_j \implies v \begin{pmatrix} 0 \\ \xi p_x + i p_y \end{pmatrix} \stackrel{(\xi p_x - i p_y)}{0} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = E \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$



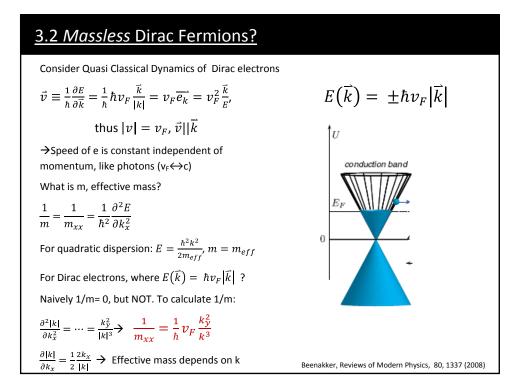


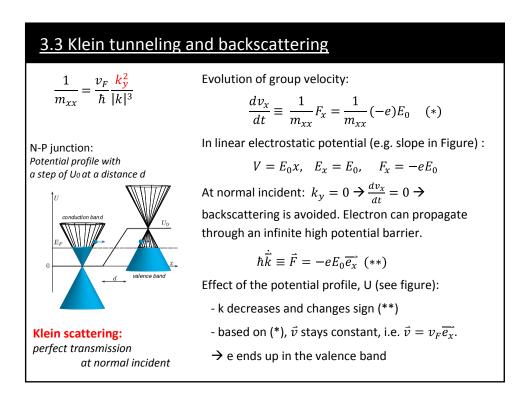


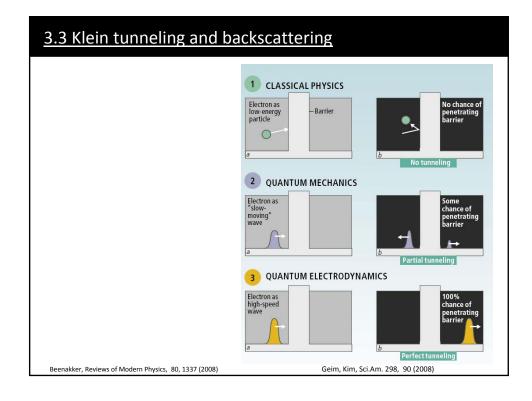
Basic transport characteristics

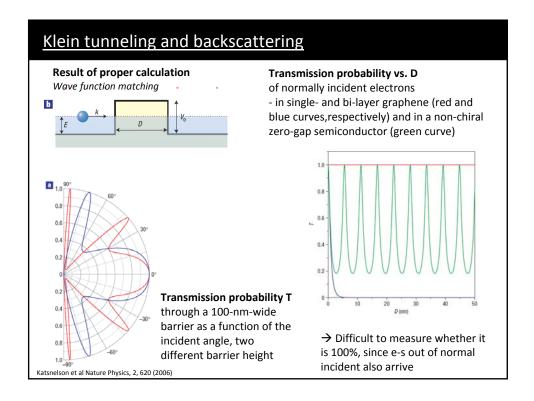


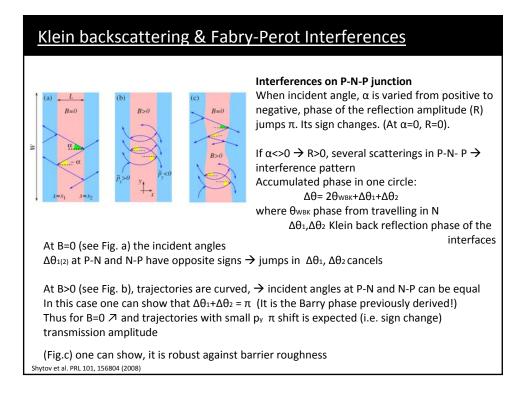
<u>3 Consequences of Dirac like spectrum 3.1 Berry's phase π</u>			
Massless Dirac fermions with Berry's phase π		$H = v \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} = v p \begin{pmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix};$	
	Solution:	<i>E</i> =	$vp \iff \psi(\varphi) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi/2} \\ e^{i\varphi/2} \end{pmatrix}$
E P _y P _y	$E = v p $ $\Psi = \frac{1}{\sqrt{2}} \left(\begin{array}{c} e^{-i\phi/2} \\ e^{i\phi/2} \end{array} \right)$ $\phi \rightarrow \phi + 2\pi$ $\Psi \rightarrow e^{i\pi}\Psi$)e ^{ip.r}	Making a loop around k=0 induces a phase shift of π . Similar to the 360° rotation of an 1/2 e spin.

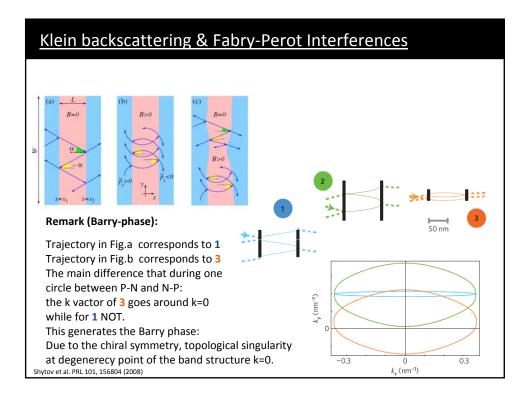


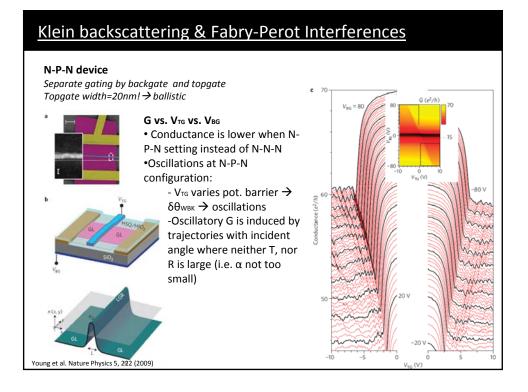


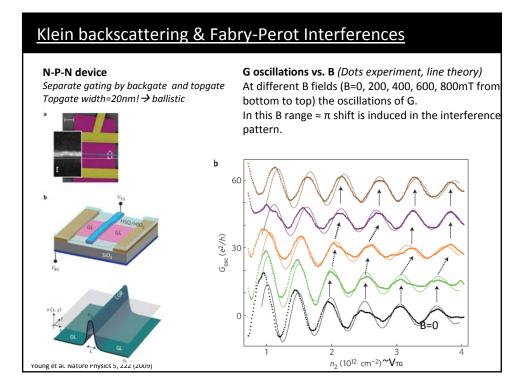


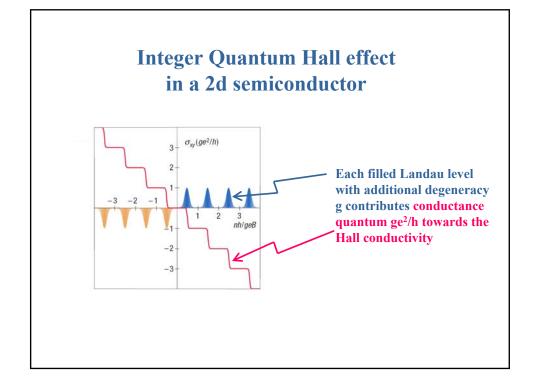


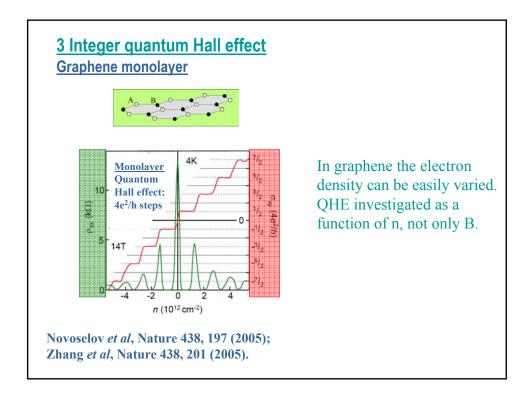


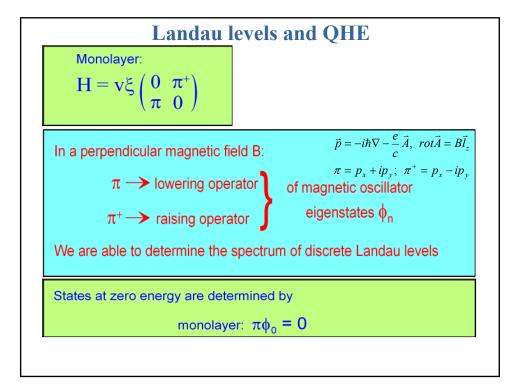


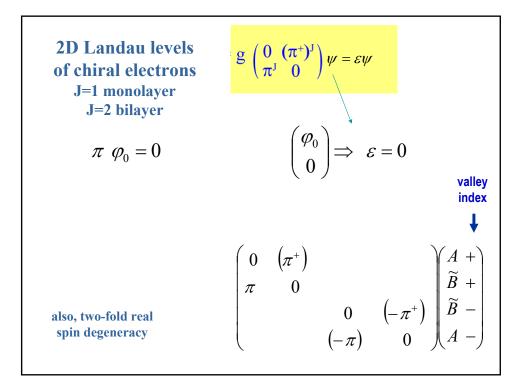


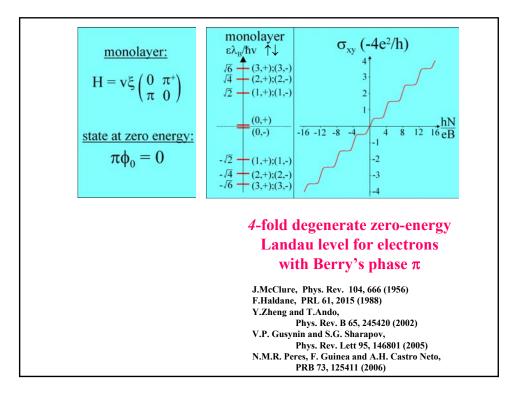


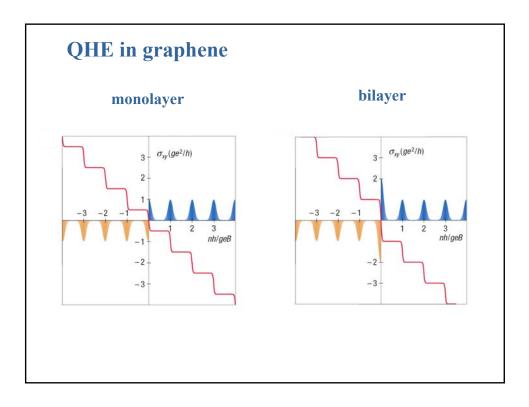


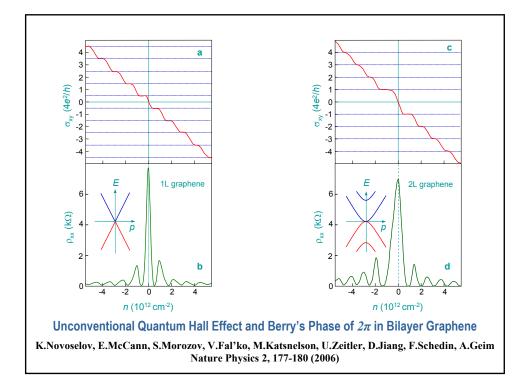


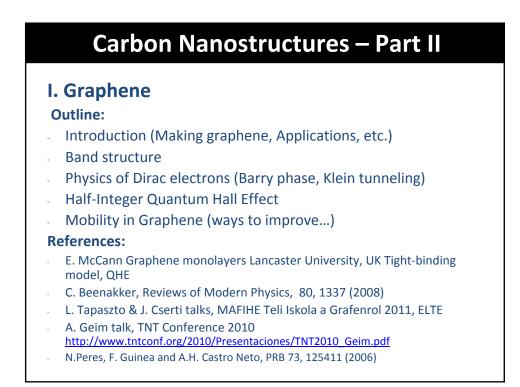


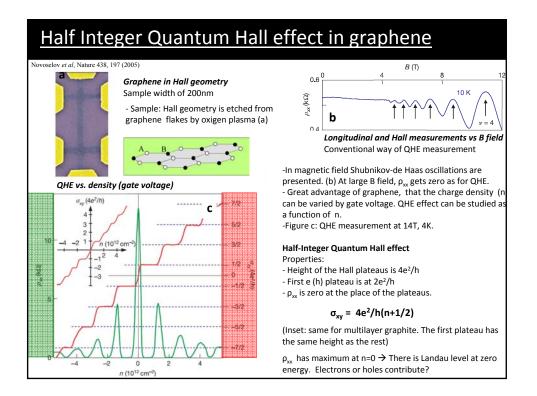












Half Integer Quantum Hall effect in graphene

Solution of the graphene Hamiltonian in B field

Let us start with the effective Dirac Hamiltonian at the K point

$$H = v \begin{pmatrix} \pi^+ \\ \pi \end{pmatrix}, \qquad \pi = p_x + i p_y, \quad \pi^+ = p_x - i p_y.$$

Hint: Besides a constant π and π^+ are the same operators as the raising and lowering operators of the harmonic oscillator Hamiltonian of the normal 2DEG in B field, i.e. $\hat{H} = \hbar \omega_c (\hat{a}^* \hat{a} + \frac{1}{2}).$

In case of magnetic field: $\vec{p} = \frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} \vec{A}$, $\vec{\nabla} \times \vec{A} = B \vec{e_z}$ Let us use a gauge of $\vec{A} = (-By, 0, 0)$: $\pi = \frac{\hbar}{i} \partial_x + \frac{e}{c} By + \hbar \partial_y$, $\pi^+ = \frac{\hbar}{i} \partial_x + \frac{e}{c} By - \hbar \partial_y$. Take the wave function ansatz, $\Psi(\vec{r}) = \begin{pmatrix} c_1 \phi_n \\ c_2 \phi_{n+1} \end{pmatrix} \frac{e^{ik_x x}}{\sqrt{L}}$: $\pi = \hbar k_x + \frac{e}{c} By + \hbar \partial_y$, $\pi^+ = \hbar k_x + \frac{e}{c} By - \hbar \partial_y$. Replacing y by y', where $\hbar k_x + \frac{e}{c} By = \frac{e}{c} By'$: $\pi = \frac{e}{c} By' + \hbar \partial_y$, $\pi^+ = \frac{e}{c} By' - \hbar \partial_y$.

Half Integer Quantum Hall effect in graphene

Solution of the graphene Hamiltonian in B field

Let us introduce a^+, a^- which fulfills the algebra of the raising and lowering operators of the harmonic oscillator: $a = \pi^+ \frac{c}{eB} \frac{1}{\sqrt{2}r_c'} a^+ = \pi^-_{eB} \frac{1}{\sqrt{2}r_c'}$ where r_c is the cyclotron radius $r_c^2 = \frac{hc}{eB}$.

It gives

$$\begin{split} a &= \frac{1}{\sqrt{2}r_c} \big(y' + r_c^2 \partial_{y'} \big), \\ a^+ &= \frac{1}{\sqrt{2}r_c} \big(y' - r_c^2 \partial_{y'} \big). \end{split}$$

These two operators fulfill: $[a, a^+] = 1$.

 ϕ_n is the eigenfunction of the a related harmonic oscillator, i.e.

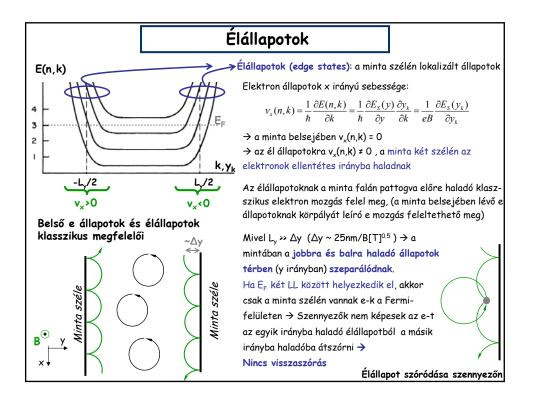
$$a|\phi_n\rangle = \sqrt{n}|\phi_{n-1}\rangle, \ a^+|\phi_n\rangle = \sqrt{n+1}|\phi_{n+1}\rangle.$$

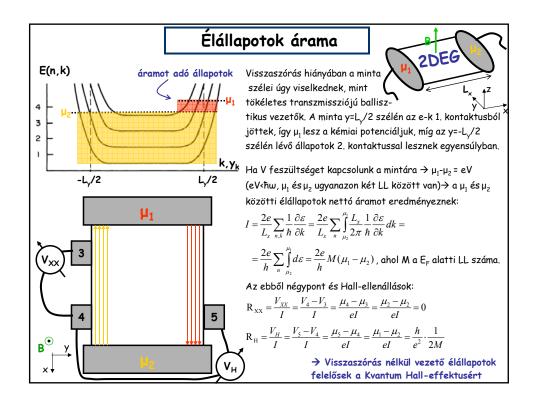
Returning to the Dirac Hamiltonian:

$$H = v \begin{pmatrix} \pi^+ \\ \pi^- \end{pmatrix} = -v \left(\frac{c}{eB} \frac{1}{\sqrt{2}r_c}\right)^{-1} \begin{pmatrix} a \\ a^+ \end{pmatrix} = -v \frac{\sqrt{2}h}{r_c} \begin{pmatrix} a \\ a^+ \end{pmatrix}$$

N.Peres et al., PRB 73, 125411 (2006)

Half Integer Quantum Hall effect in graphene Solution of the Hamiltonian of Dirac electrons in B field Let us start with the wavefunction $\Psi_n(\vec{r}) = \begin{pmatrix} \phi_n \\ \alpha \phi_{n+1} \end{pmatrix} \frac{e^{ik_{\chi}x}}{\sqrt{L}}$ where $\alpha = \pm 1$. $H\Psi_n \to \begin{pmatrix} a \\ a^+ \end{pmatrix} \begin{pmatrix} \phi_n \\ a\phi_{n+1} \end{pmatrix} = \begin{pmatrix} \sqrt{n+1}a\phi_n \\ \sqrt{n+1}\phi_{n+1} \end{pmatrix} = \sqrt{n+1}\alpha \begin{pmatrix} \phi_n \\ a\phi_{n+1} \end{pmatrix}$ $H\Psi_n = -v \frac{\sqrt{2}\hbar}{r_c} \sqrt{n+1} \alpha \Psi_n$ Landau levels in graphene: $E_n = \pm v \frac{\sqrt{2h}}{r_c} \sqrt{n+1}, \quad n = 0, 1, 2, ...$ There is an extra solution as well: $\Psi_0 = \begin{pmatrix} 0 \\ \phi_0 \end{pmatrix} \frac{e^{ik_x x}}{\sqrt{L}}$. $H\Psi_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = E\Psi_0 \rightarrow E_0 = 0$. Degeneracy of the levels: Similar to normal Landau Levels. $L > y > 0 \rightarrow L > \frac{hc}{eB}k_x > 0$ and $k_x = \frac{2\pi}{L}n$ where n is integer. → The degeneracy: $N = \frac{L^2 B/c}{h/e}$ i.e. number of flux quantum Density of states ΛD penetrating the sample. B=0 Solving the problem for the K' effective Hamiltonian Ę gives the same spectrum as the one for K. Therefore ↑ D each E_n energy level has a degeneracy of N * 2 * 2. B>0 2 from the two valleys, 2 from the real spin of the electrons. N.Peres et al., PRB 73, 125411 (2006)





Half Integer Quantum Hall effect in graphene

Solution of the Hamiltonian of Dirac electrons in B field

Remark:

The edge states behave similar to the ones of QHE of normal 2DEGs.

$$v_{\chi} = \frac{1}{\hbar} \frac{\partial E}{\partial k_{\chi}} = \frac{1}{\hbar} \frac{\partial E}{\partial y} \frac{\partial y}{\partial k_{\chi}} = \frac{1}{\hbar} \frac{\partial E}{\partial y} \frac{1}{eB/c}$$

On the two sides of the sample they propagate to opposite direction.

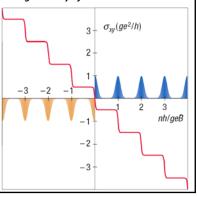
Half-integer quantum Hall-effect:

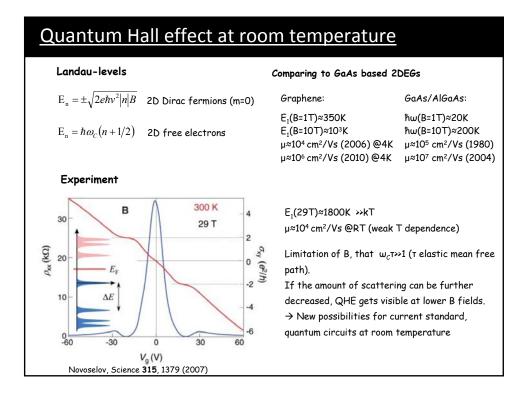
Charge density of Landau levels

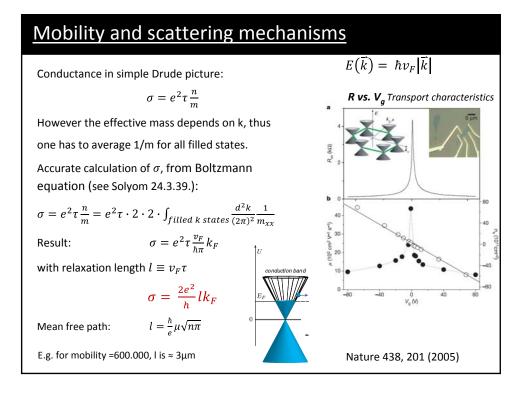
Due to the 2 spin and 2 valley, there are 4-fold degenerate Landau levels. Each degeneracy provides a conductance channel with $G = \frac{e^2}{h}$. Therefore each filled LL enhance the Hall conductance by $G = \frac{2:2\cdot e^2}{h}$. When E_F is placed on a LL, the Hall conductance changes from a quantized plateau to the next one. Since there is a LL at ZERO ENERGY the first electron like Hall plateau is at $G = \frac{2\cdot e^2}{h}$ and the rest are at $G = \frac{2\cdot 2\cdot e^2}{h} (n + \frac{1}{2})$. The zero energy LL makes the QHE of graphene special.

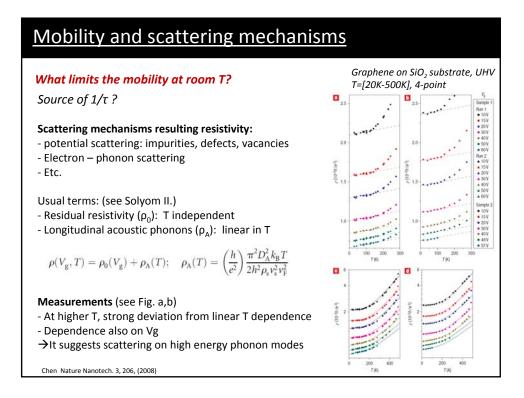
The zero energy LL makes the QHE of graphene special. It consist e and hole states as well.

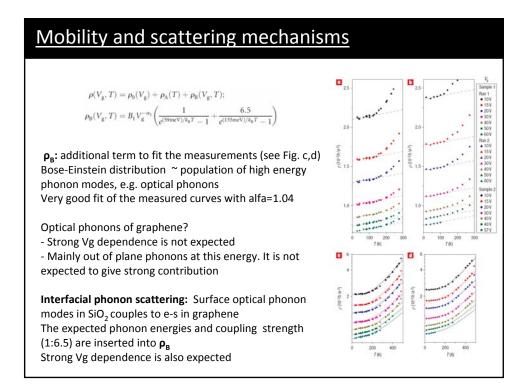
N.Peres et al., PRB 73, 125411 (2006)



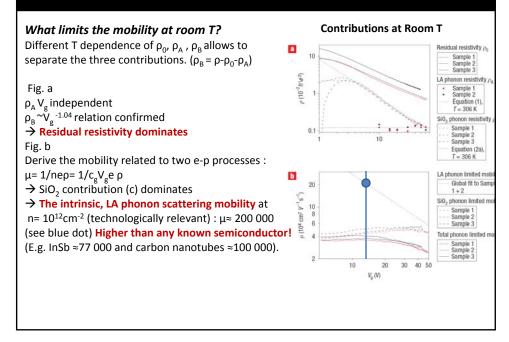


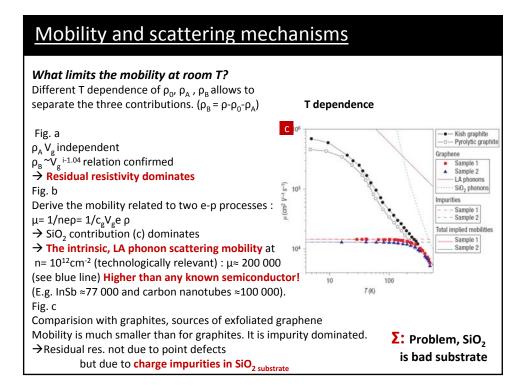


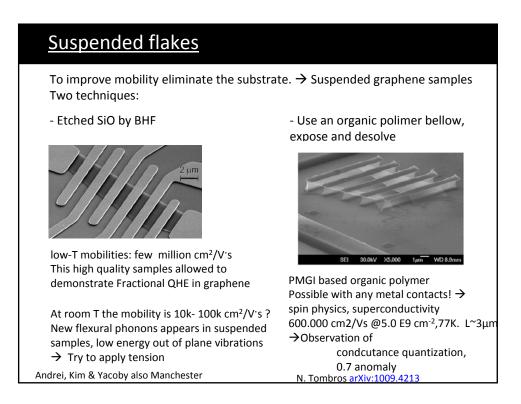


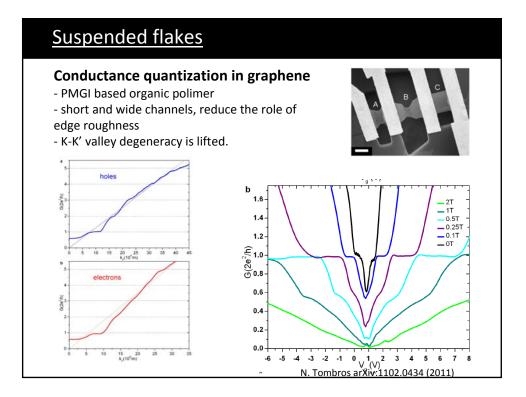


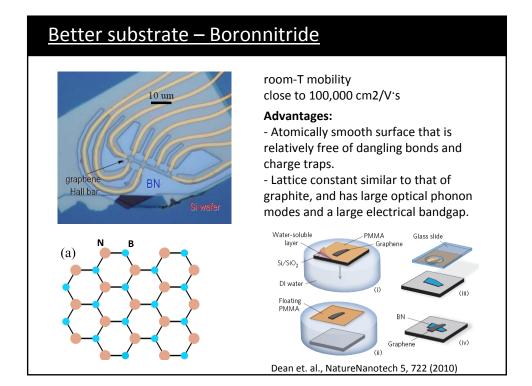
Mobility and scattering mechanisms

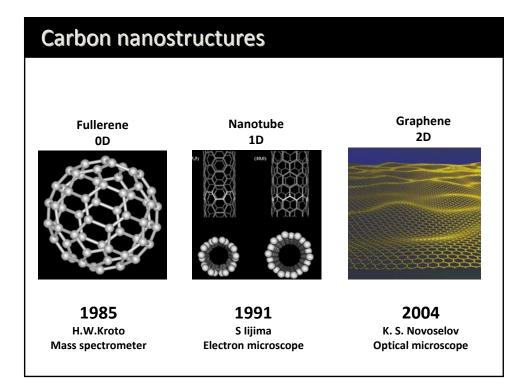




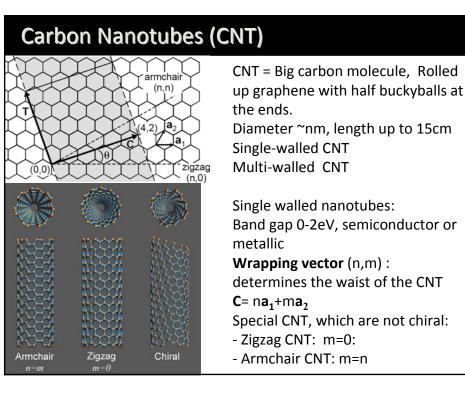


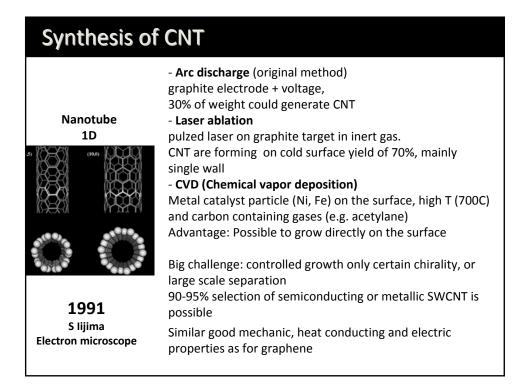




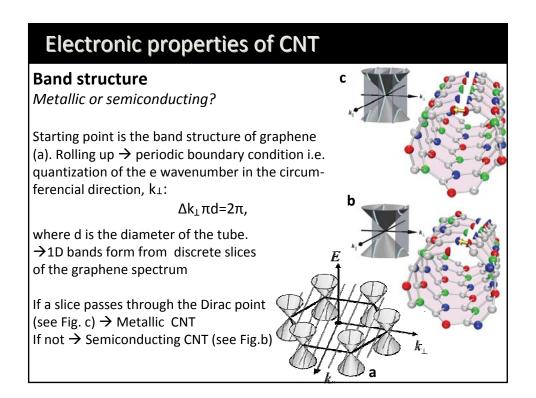


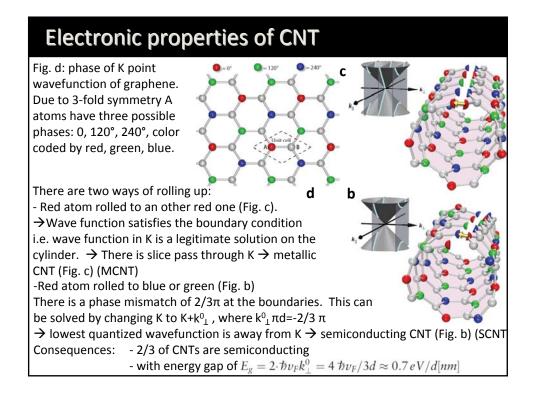
	Carbon Nanostructures
П	. Carbon Nanotubes (CNT)
C	Outline:
-	Single walled carbon nanotubes (wrapping)
-	Synthesis
-	Electronic properties (metallic vs. semiconducting CNT)
-	Quantum transport (Ballistic conductance, Fabry-Perot interference)
-	CNT Quantum dots (spin, orbital degeneracy, Orbital and SU(4) Kondo effect)
Re	eferences:
-	S Ilani and P. L. McEuen Annu. Rev. Condens. Matter Phys 1, 1–25 2010. and references within.
-	P. Jarillo-Herrero, Quantum transport in carbon nanotubes, phd thesis 2005. Wikipedia: en.wikipedia.org/wiki/Carbon_nanotubes





KomplexNano





Electronic properties of CNT

In reality usual metallic tubes also shows **small bandgap**. Since the metallic band structure is instable against perturbation like e.g. mechanical deformation. Everything what destroys A⇔B symmetry (i.e. pseudospin) generates gap. Taken into account the curvature of small diameter CNTs also generates gap.

Figures: measured transport characteristics @RT. Gate electrode is used to change the e filling.

Maximal conductance:

In Landauer picture each ballistic subband gives a maximal conductance of e^2/h . In CNT there are 4 subbands, due to 2 spin and 2 isospin (valley K, K') degeneracies. I.e. $G_{max}=4e^2/h$.

The conductance is also limited by contact resistances. $v_{\rm G}(v)$ It has to be a clear transparent barrier. For semiconductor tubes palladium gives Schottky-barrier free contacts for p-type CNTs. While Al with low work function gives good contact to n-type CNTs.

Semiconducting

Small bandgap

0.15

G(e²/h)

Off state

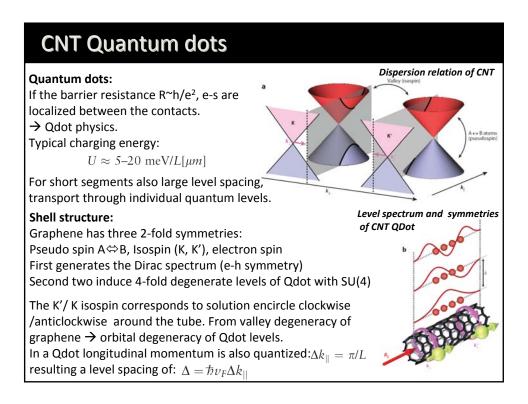
Off state

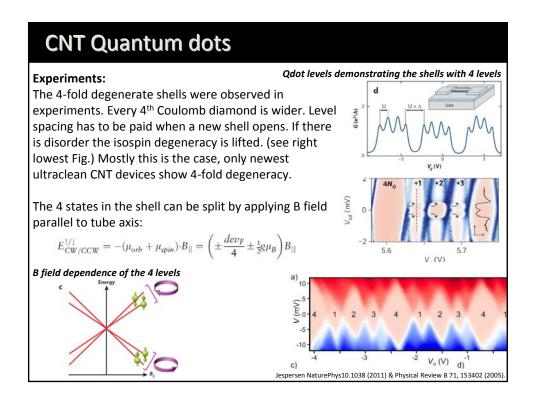
VG(V)

Electronic properties of CNT Typical numbers of mean free path and mobility: Semiconducting I ~100nm (SCNT) ~1μm (MCNT) @RoomT and μ>100.000 cm²/Vs (SCNT), l_e ~10μm (MCNT) @<50K G(e²/h) The large mean free path has the same origin as for graphene. C has light mass, sp² is a strong bonds \rightarrow Off state high energy phonons, which are only populated at high T. V_G(V) Small bandgap 0.15 Limit of maximal current At large source drain biases, e-s accelerate in the G(e²/h) tube and can excite optical zone boundary phonons. This dramatically decrease l to 10nm, and thereby Off state this voltage threshold limits the current: I_{max} ~ 4e²/h $\hbar \omega_0$ /e~25 μ A $\hbar\omega_0 = 160 \text{meV}.$ $V_{G}(V)$

Quantum transport of CNT

Sample geometry with electron path G vs. V_a and Bias (mV) Ballistic and coherent transport scattered on the contact interfaces at low T (T<5K) **Fabry-Perot cavity** Due to coherent scattering on Corresponding scattering the imperfect contacts matrix problem interferences occur: periodic oscillations as a function of gate V o and bias. $V_{\rm g}$ or bias changes kand thereby the accumulated phase on one loop. Periodicity of the oscillations vs. Length of the CNT segment Periodicity (V_c) is proportional periodicity determined by to L⁻¹, where L is the length of arrow position in right figure CNT segment. (mV) n (4/20) AP/IP / -1 (um-1

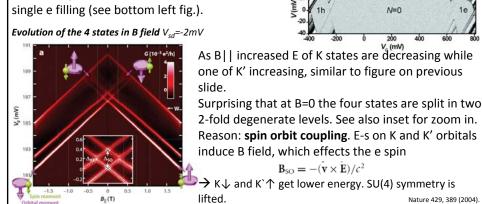




CNT Quantum dots

In semiconducting CNTs one can access the single electron and single hole filling of the quantum dot (see right figs). Large diamond corresponds to the empty quantum dot.

In ultraclean CNTs (grown on top of the electrodes) shell structure was studied at single e filling (see bottom left fig.).

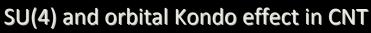


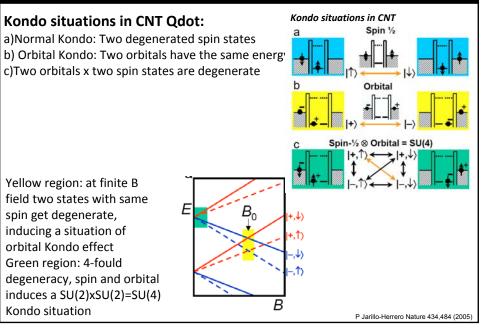
1e and 1 hole state of semiconducting CNTs

T=0.3 K

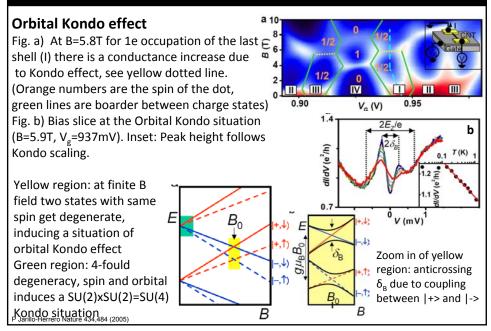
V.M

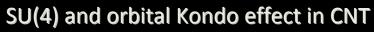
V_c(V)





SU(4) and orbital Kondo effect in CNT





SU(4) Kondo effect signatures Fig. a) Decreasing T, G increases in the

valley of state I and III. Fig. b) B=0 zero bias resonance appears

in state I and III. (There is no orbital splitting as in previous slide due to higher Kondo temperature $\delta_{B} < T_{\kappa}$)

Fig. c) At B=1.5T the Kondo resonance splits into 4 branches for state I

Fig. d) The splitting of the 4 states vs. B field for state I.

Outer lines are cotunneling from |-> to |+> orbitals, while the inner lines are cotunneling process from |-, \uparrow >

to $|-, \downarrow >$. ($\mu_{spin} = \mu_B$, $\mu_{orbital} = 13\mu_B$) The multiple splitting provides direct evidence of the SU(4) Kondo

resonance.

(For B=1.5T & III the inner two states are not split. Since T_k large spin-1/2 SU(2) Kondo remains.)

