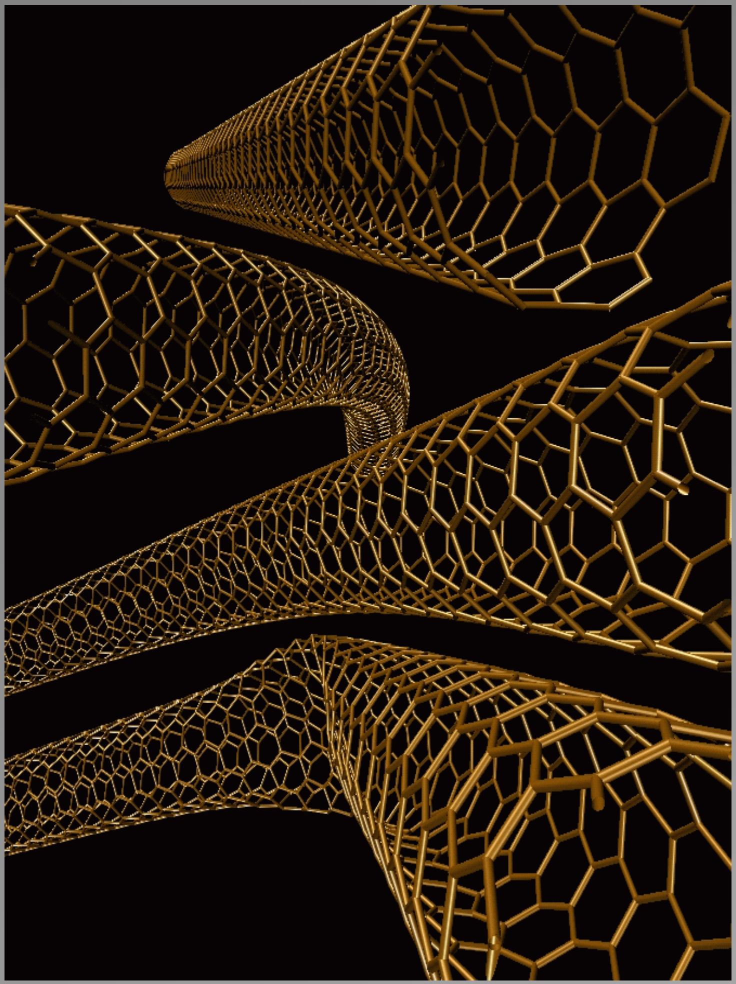
Regensburg, 20.07.2005



Orbital magnetic moment in pure and doped carbon nanotubes

Magdalena Margańska

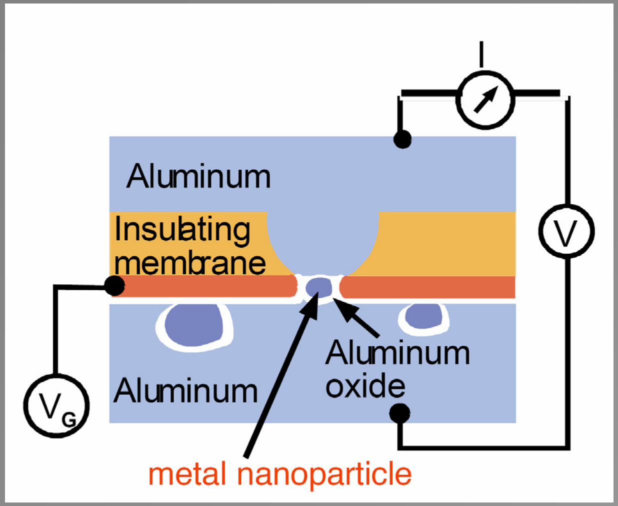
Institute of Theoretical Physics, University of Silesia

in collaboration with: M. Szopa, E. Zipper

Contents

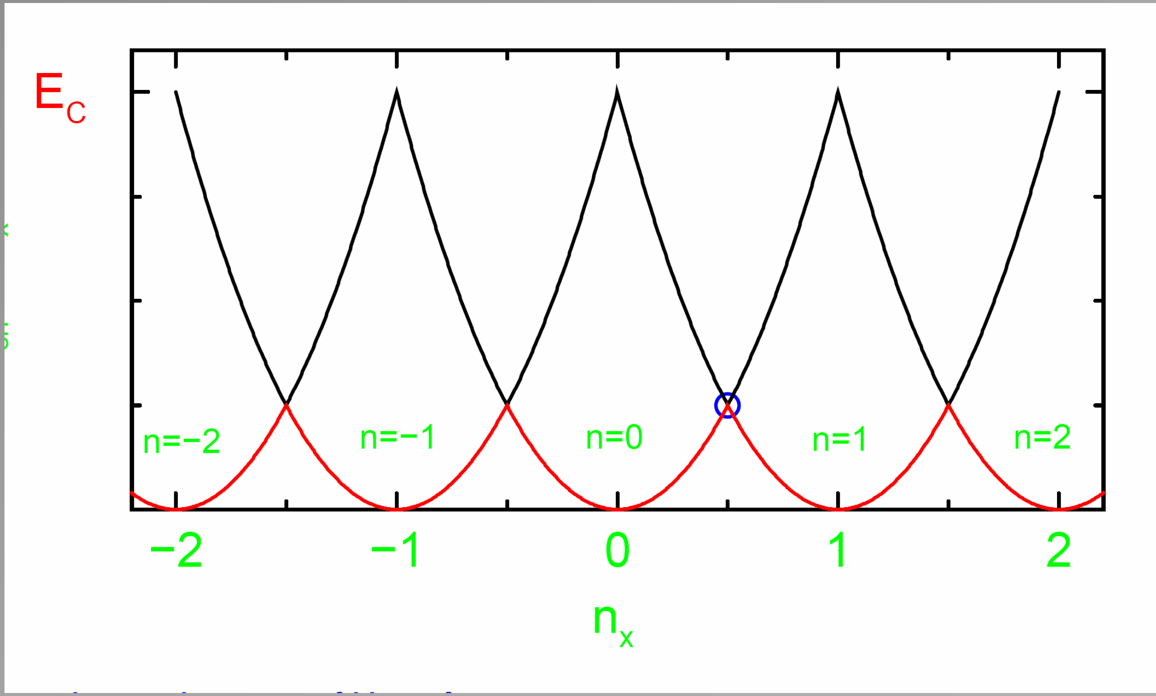
- Carbon and inorganic nanotubes
- Aharonov-Bohm effect and persistent currents
- Magnetic moment – of an electron or of a nanotube?
- Magnetic moment of a single-wall nanotube, pure and doped
- The question of the true shape of the dispersion relation
- Orbital magnetic moment of a multiwall nanotube
- Collective effects

Coulomb blockade in a quantum dot



- Condensator charging energy

$$E = \frac{Q^2}{2C}$$



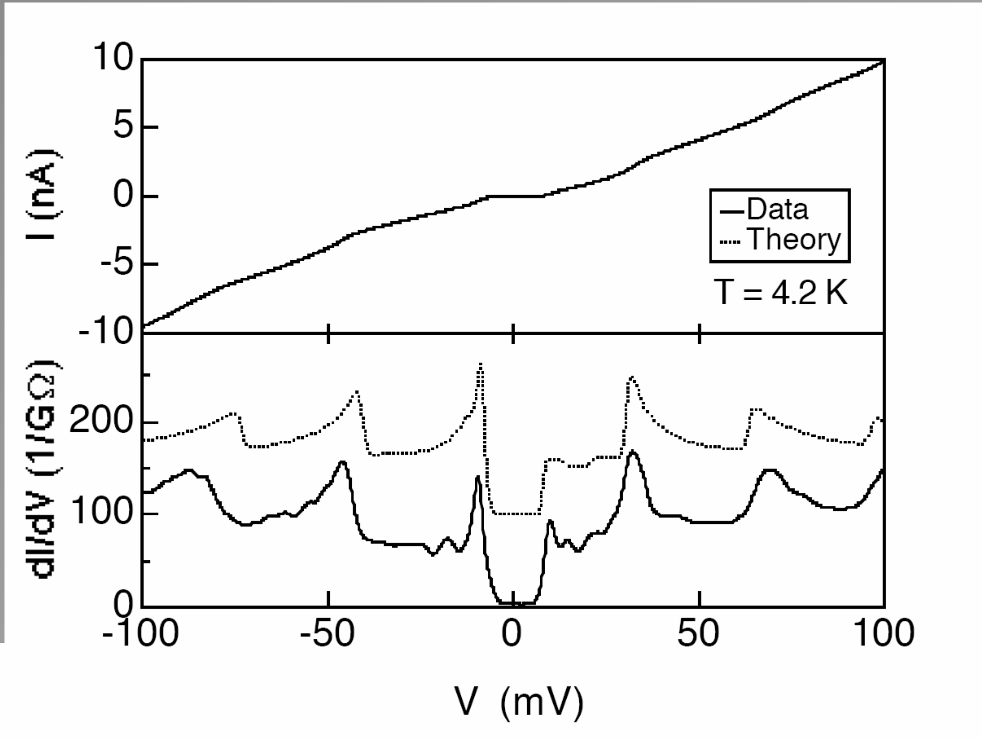
Energy of an n-electron quantum dot

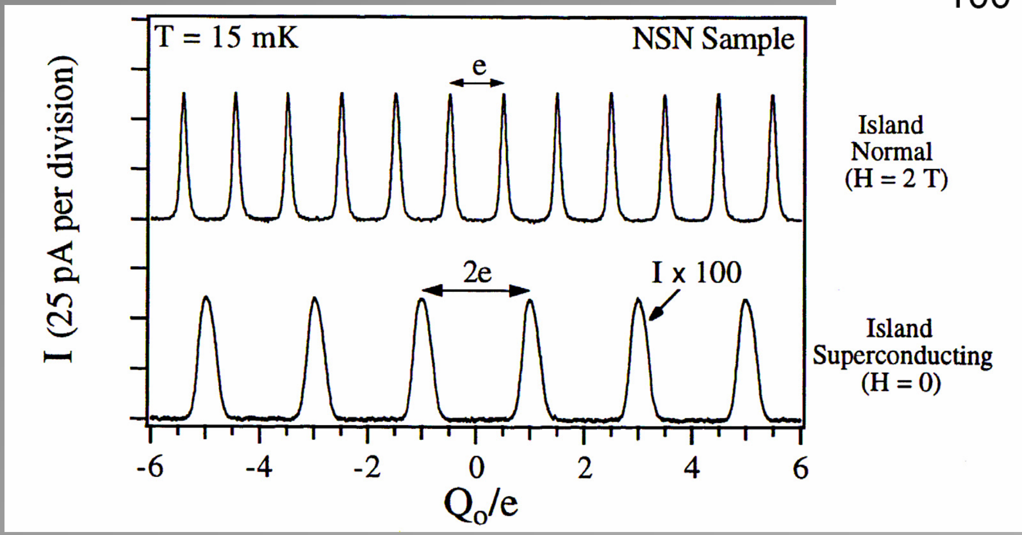
$$E(n) = \frac{(ne - V_g C_g)^2}{2C}$$

D.Ralph, J. Konig, Les Houches 2004

Current-voltage characteristics of a quantum dot

The conductance of a state sharply increases when the energy of the n-electron state is the same as of the n+1-electron state.

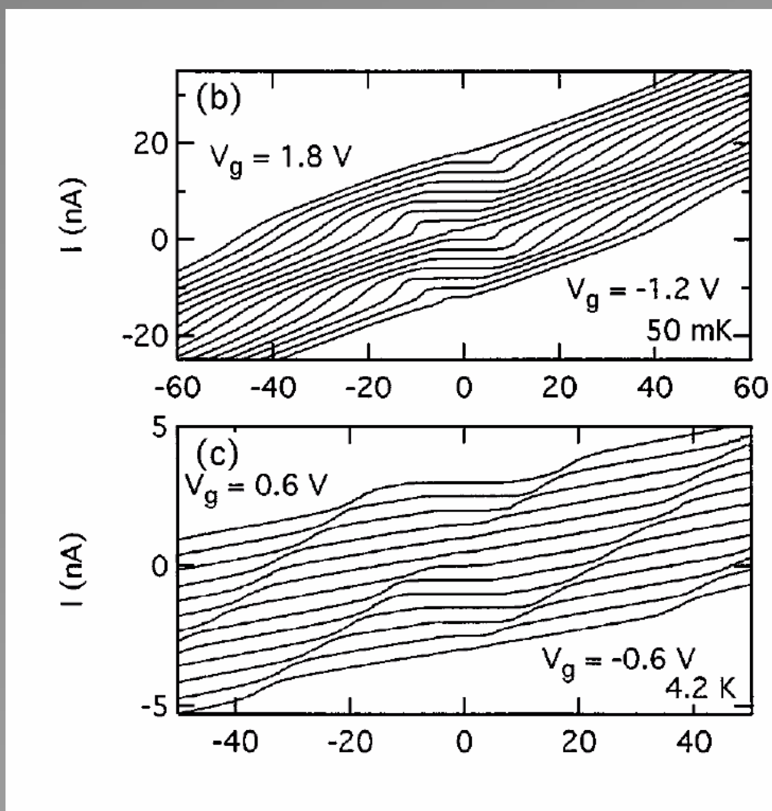


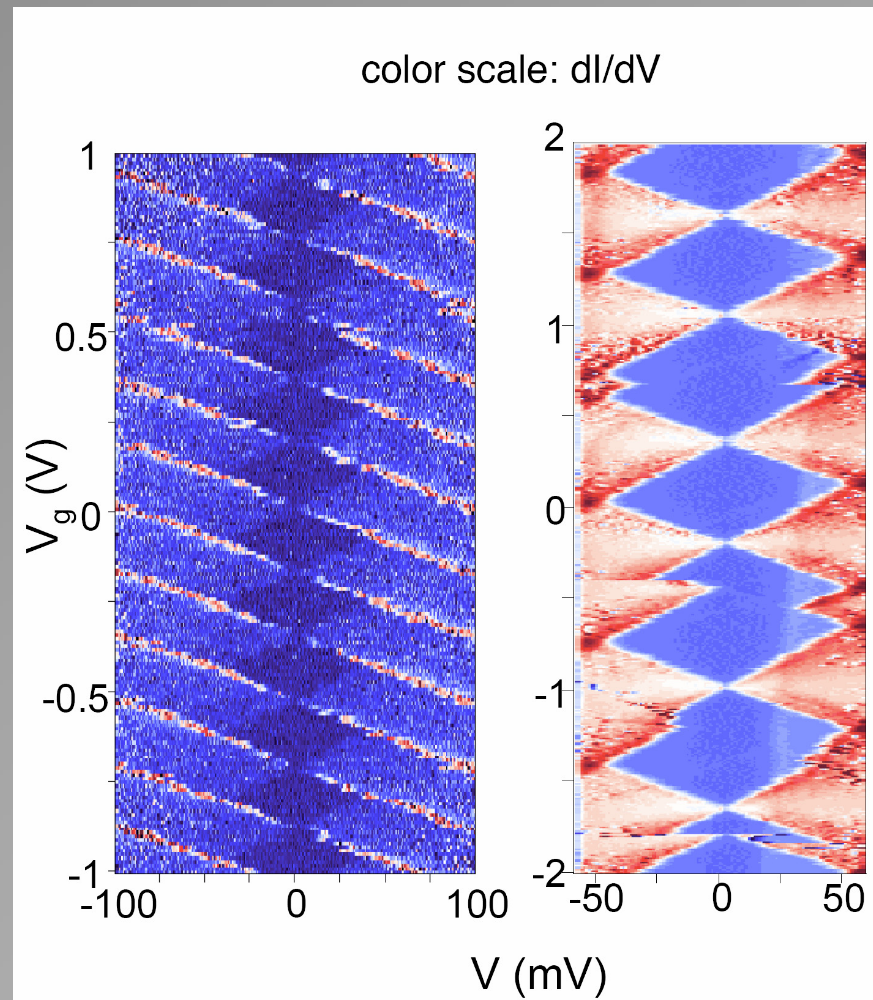


Differential conductance dI/dV

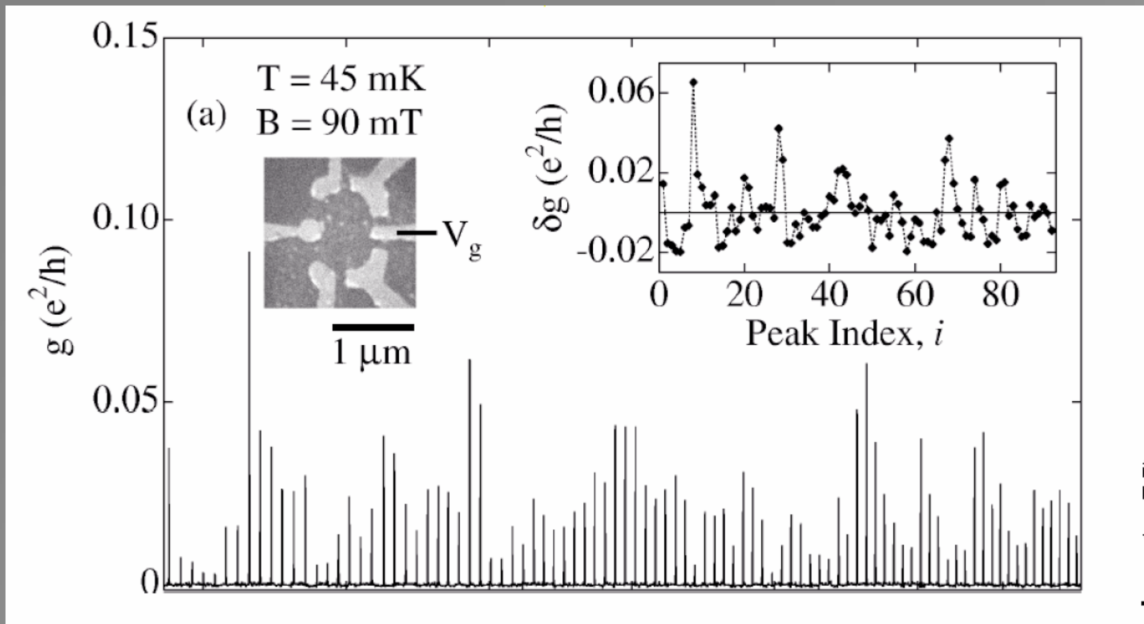
Quantum dot conductance can be controlled by the gate voltage.

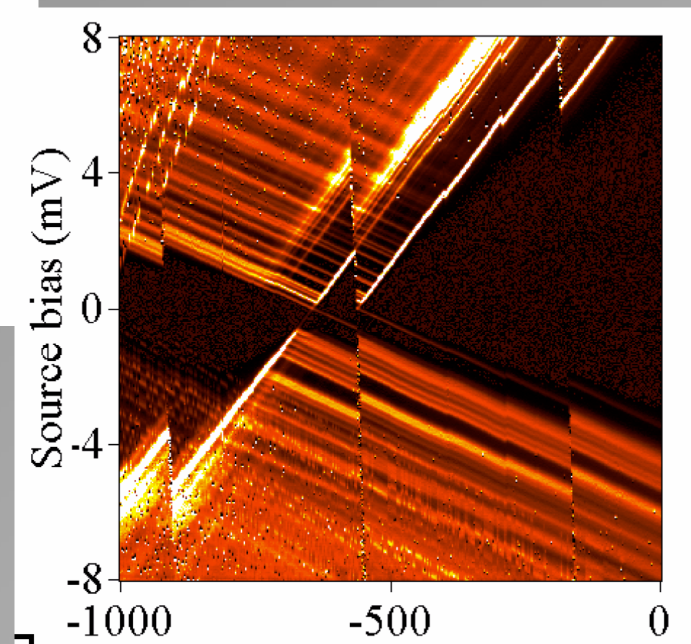
$$\left(E(n) = \frac{(ne - V_g C_g)^2}{2C} \right)$$

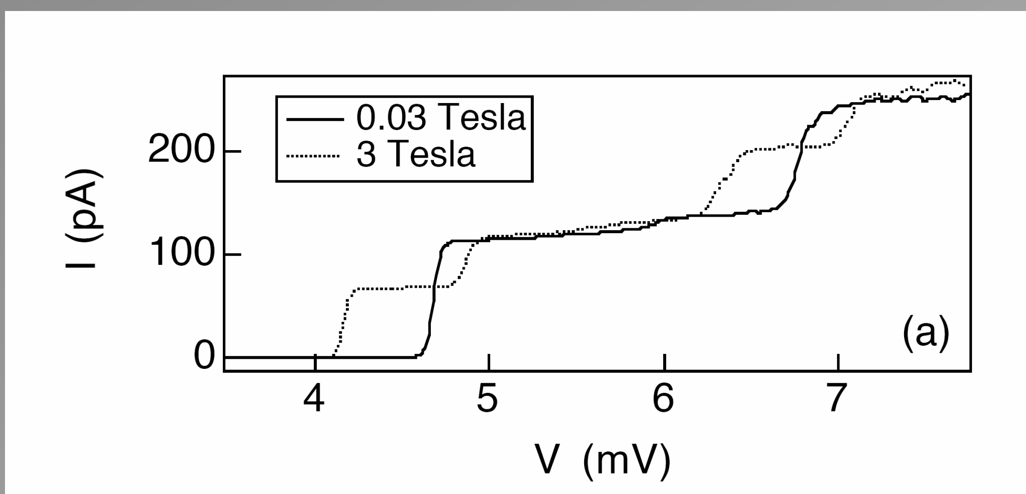




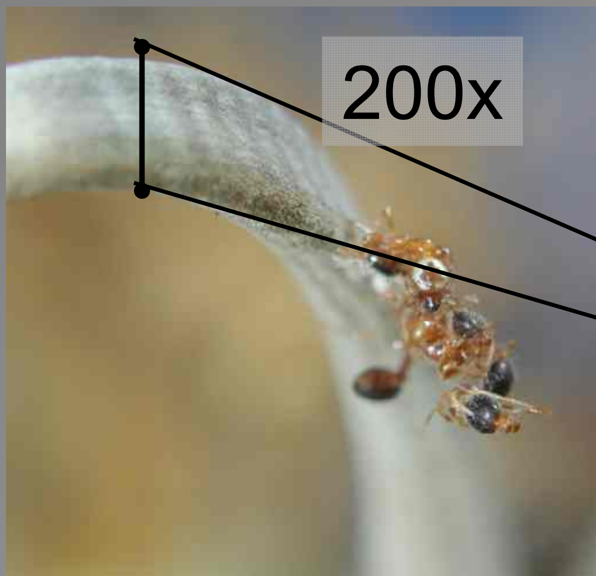
Coulomb blockade – discrete levels

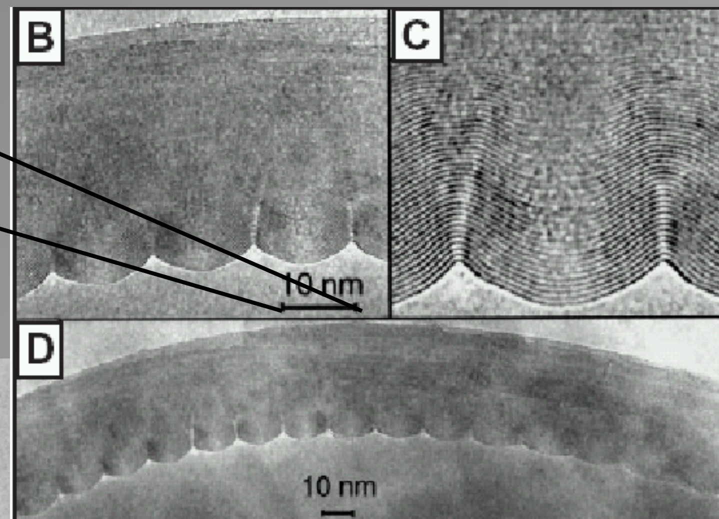


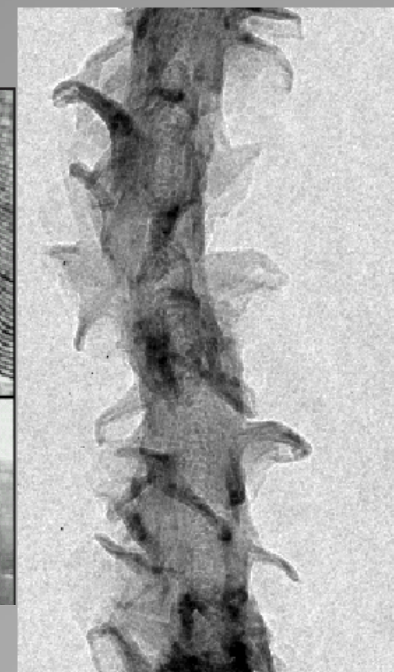


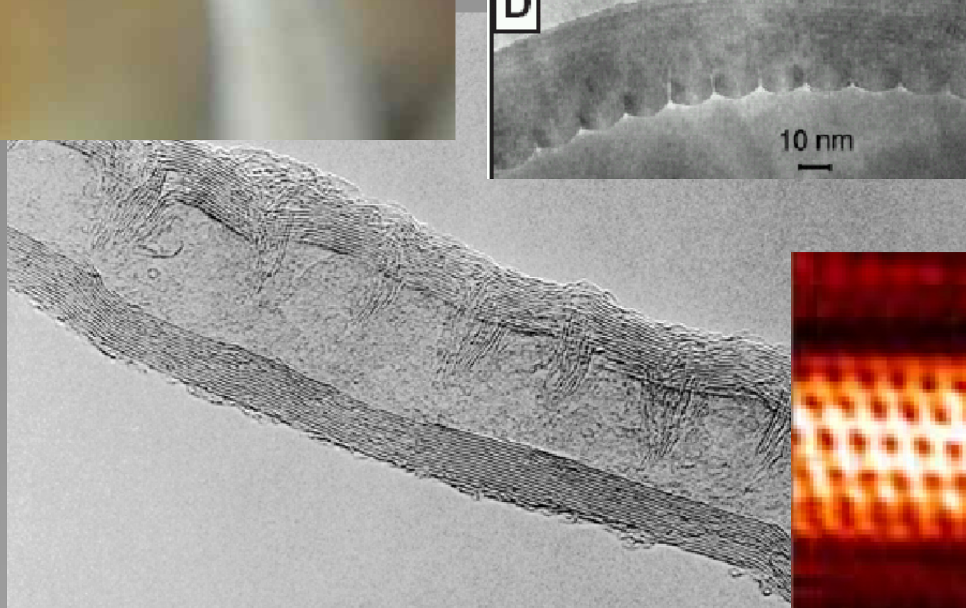


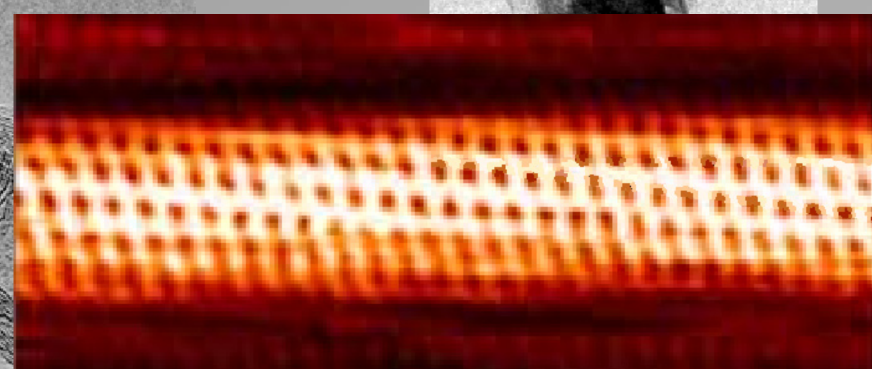
Carbon nanotubes



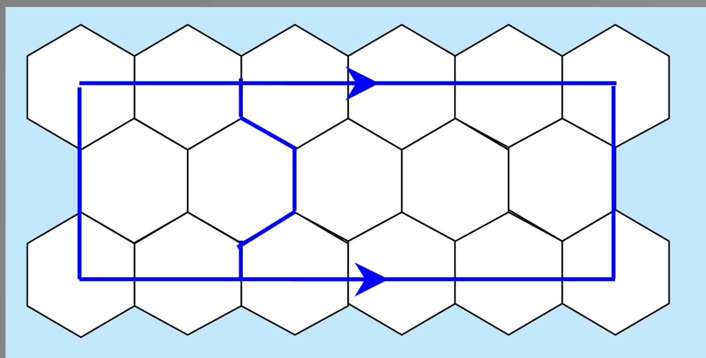


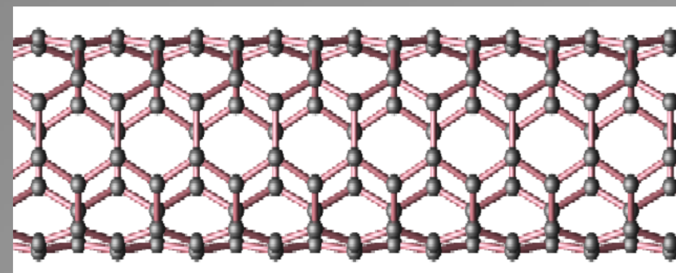




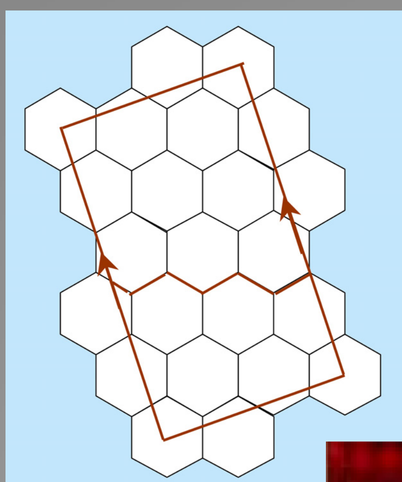


Nanotube types

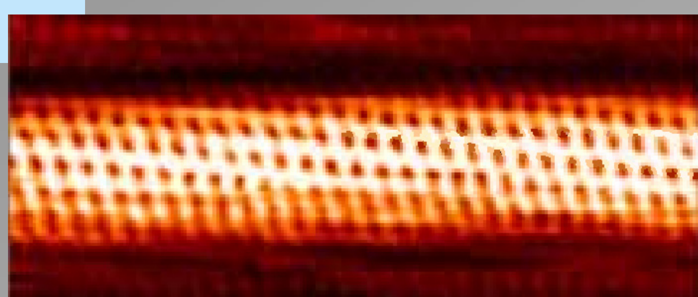


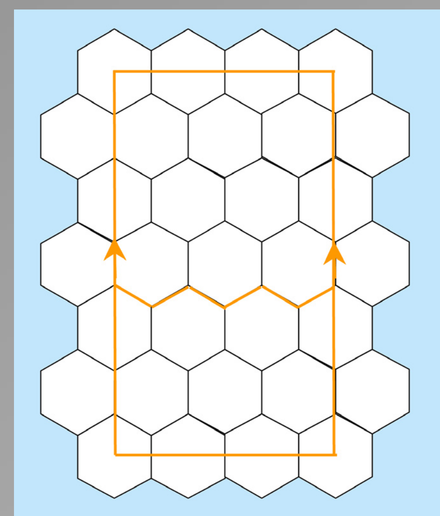


Armchair

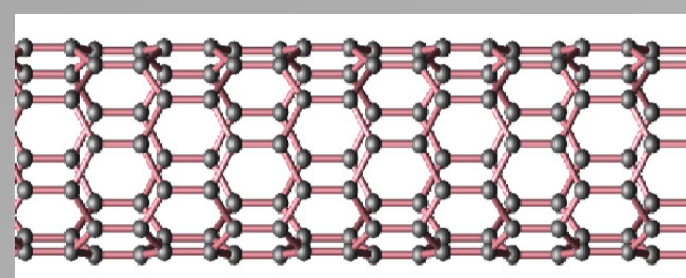


Chiral

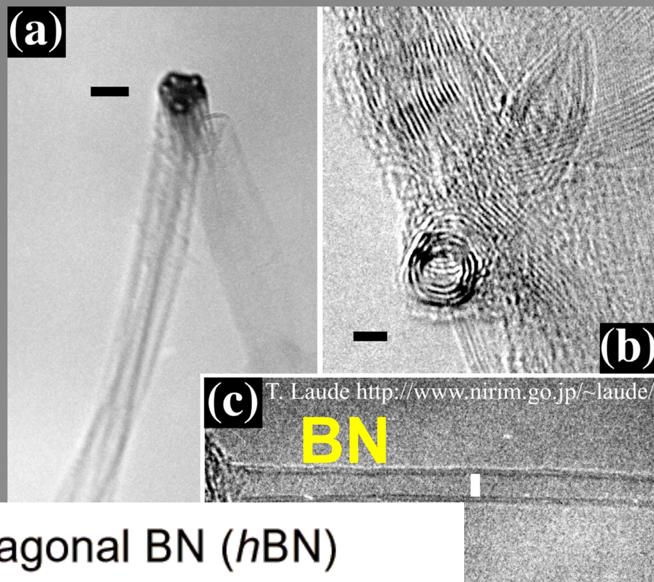


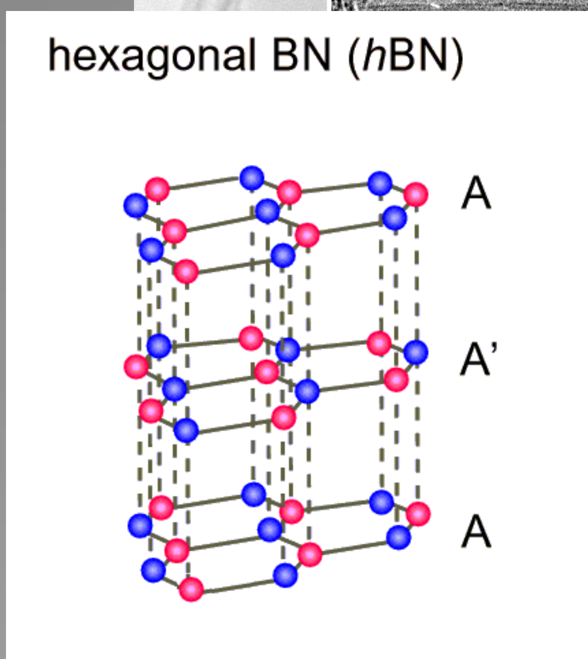


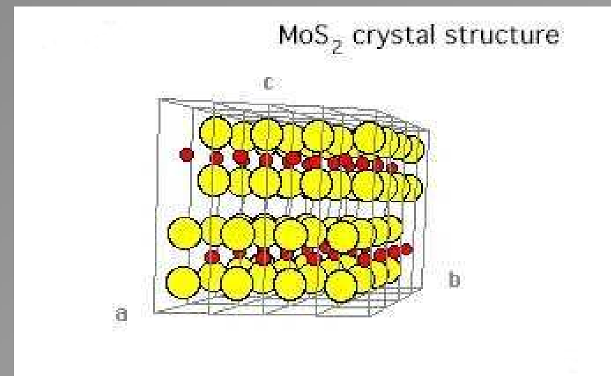
Zigzag

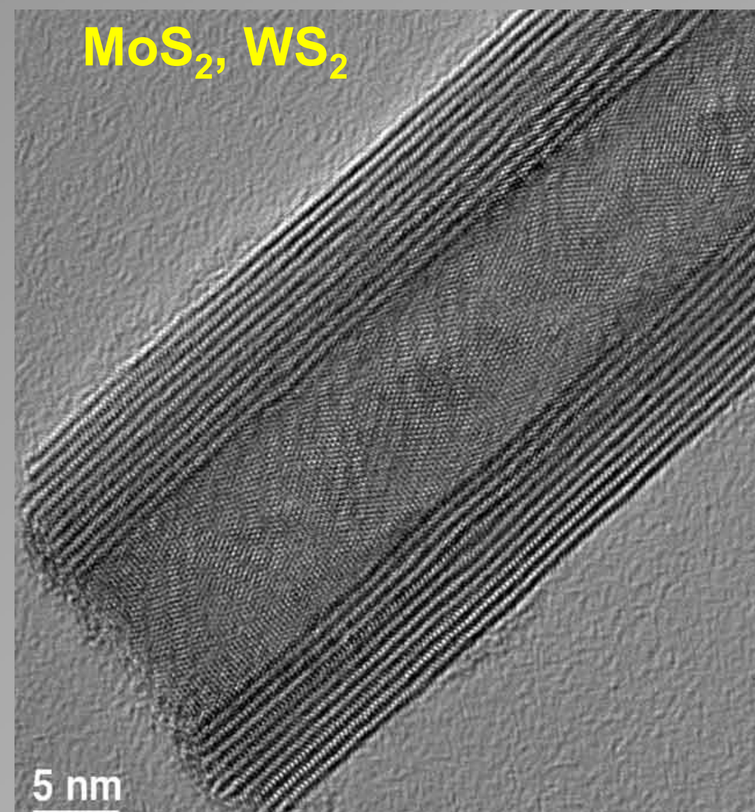


Inorganic nanotubes



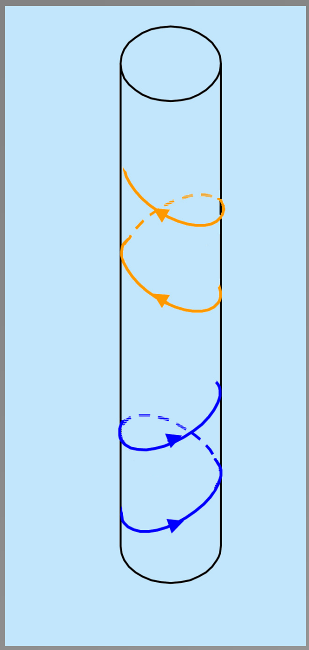






Aharonov-Bohm effect and persistent currents

Vector potential modifies boundary conditions:



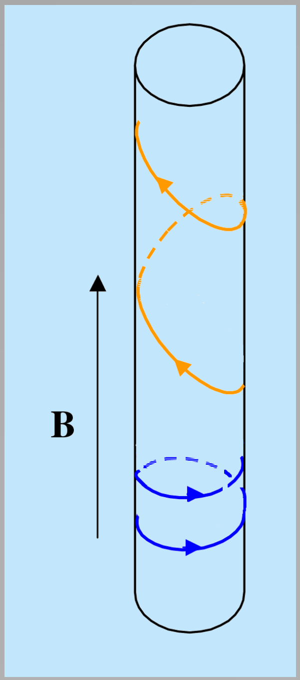
$$\exp(ikL) \;\rightarrow\; \exp\left(\frac{i}{\hbar}\oint(\mathbf{p}-e\mathbf{A})\cdot \mathrm{d}\mathbf{r}\right) = \exp\left(ikL - i\frac{e}{\hbar}\int \mathbf{B}\cdot \mathrm{d}\mathbf{S}\right) =$$
$$= \exp\left(ikL + i\frac{e}{\hbar}\phi\right) = \exp\left(i2\pi(n+\frac{\phi}{\phi_0})\right),$$

Momentum states are shifted in the direction perpendicular to the magnetic field

$$\mathbf{k}\cdot\mathbf{L}_\perp = 2\pi(l_\perp + \frac{\phi}{\phi_0}), \qquad l_\perp \in \mathbb{Z},$$

Each electron carries the current given by

$$I_\mathbf{k}(\phi) = -\frac{\partial E_\mathbf{k}}{\partial \phi} = -\frac{\partial E_\mathbf{k}}{\partial k_l}\frac{\partial k_l}{\partial \phi} = -\frac{\partial E_\mathbf{k}}{\partial k_l}\frac{2\pi}{\phi_0|\mathbf{L}_t|}$$



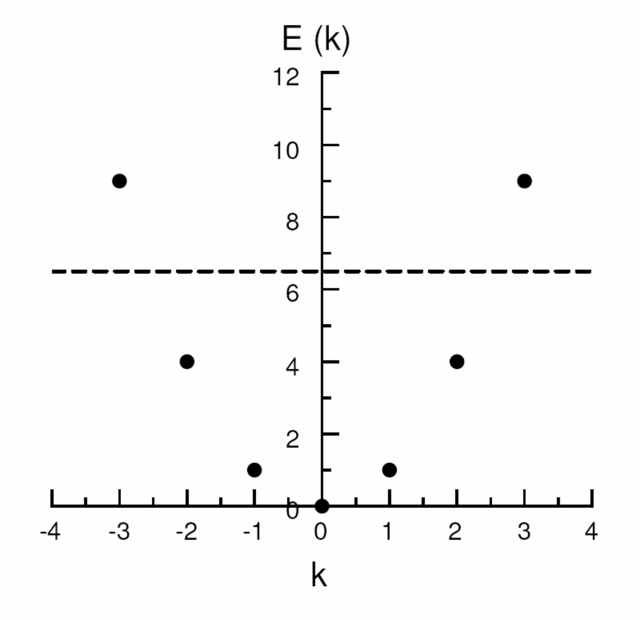
These currents don't cancel out at nonzero fields.

Persistent currents in mesoscopic rings

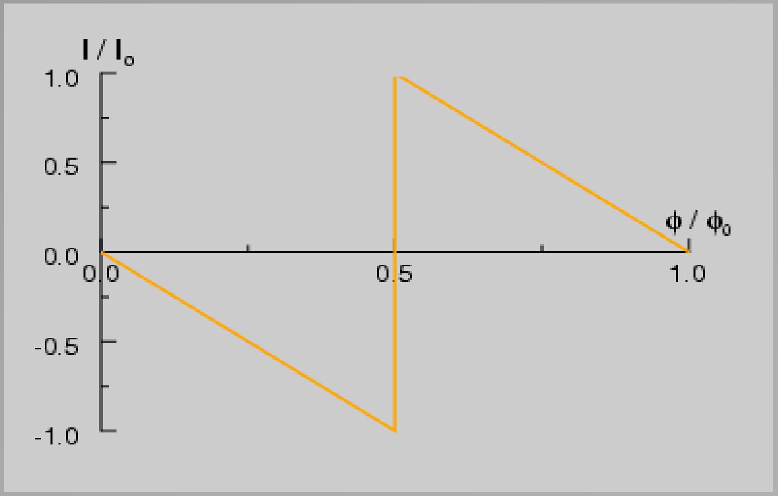
In the free electron model

$$E_n(\phi) = -\frac{p^2}{2m} = \frac{\hbar^2}{2m}\left[\frac{2\pi}{L}\left(n+\frac{\phi}{\phi_0}\right)\right]^2,$$

For odd number of electrons



B=0



Persistent currents in mesoscopic rings

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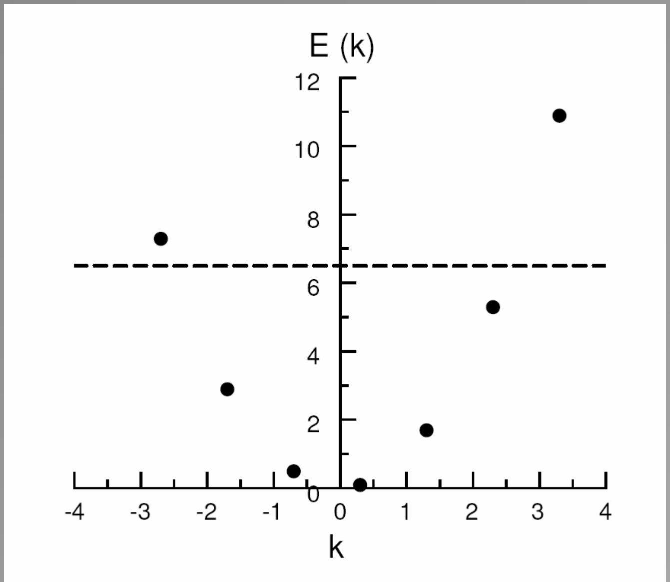
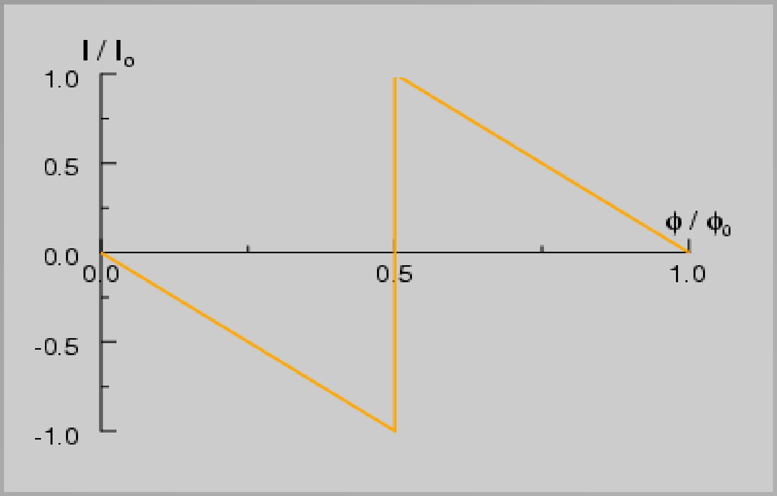
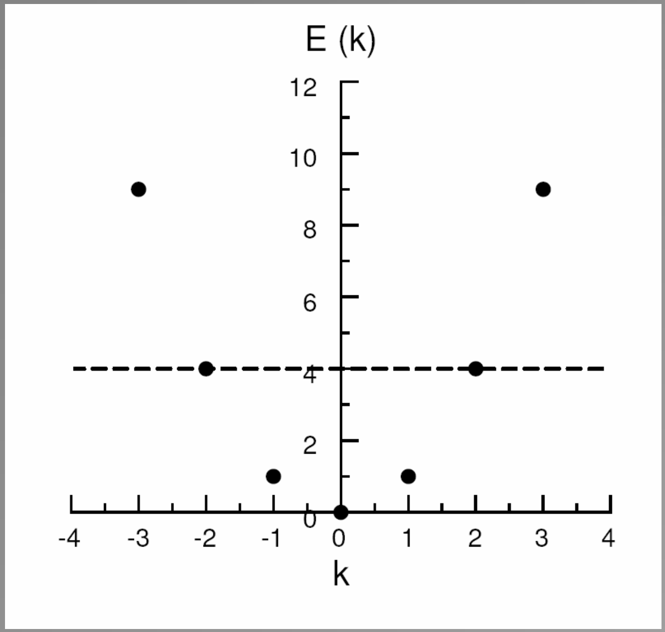


B≠0

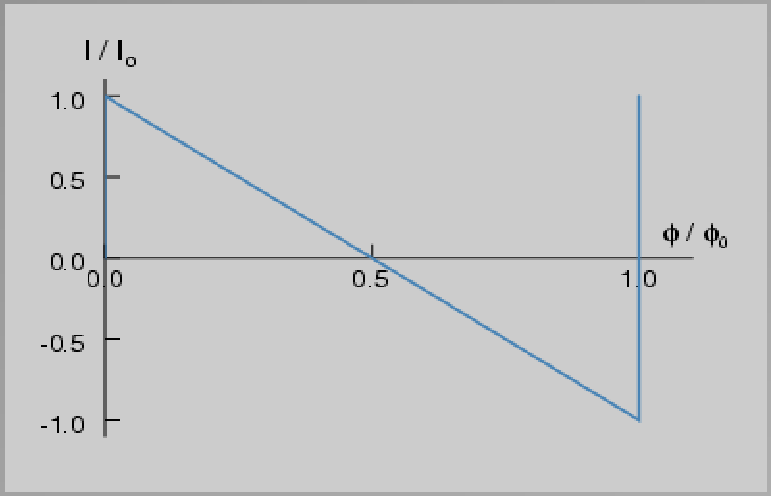


Persistent currents in mesoscopic rings

For even number of electrons



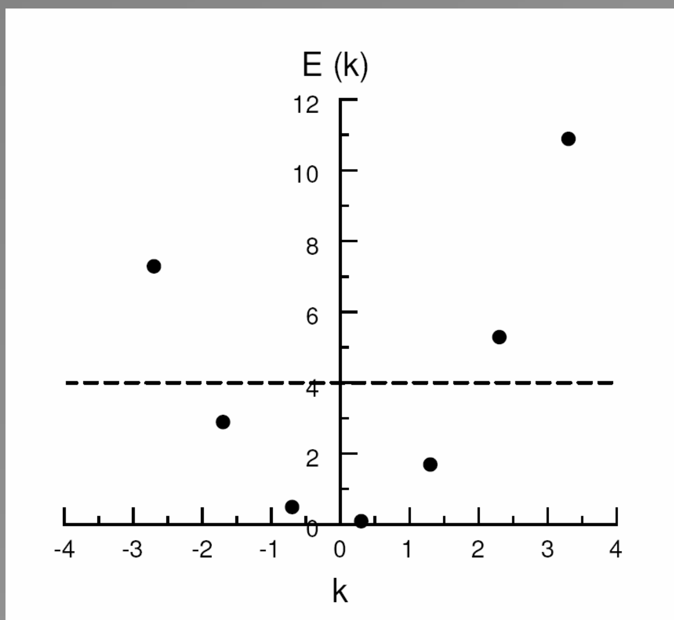
B=0



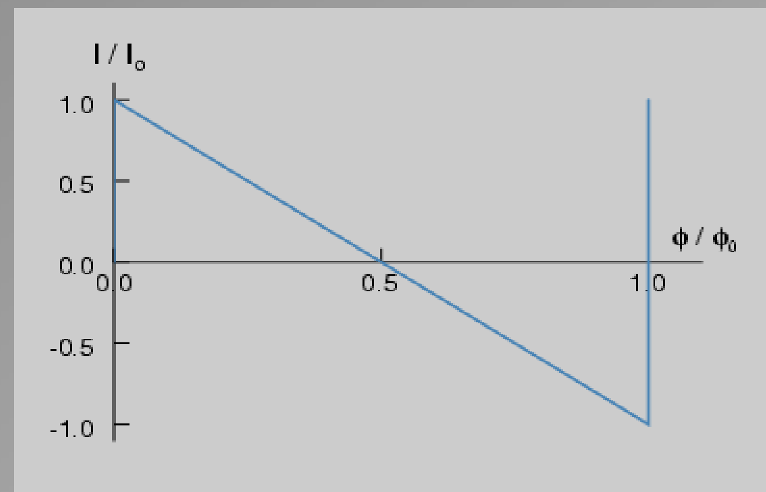
A strong paramagnetic currents appears when momentum states cross the Fermi level.

Persistent currents in mesoscopic rings

For even number of electrons



$B \neq 0$



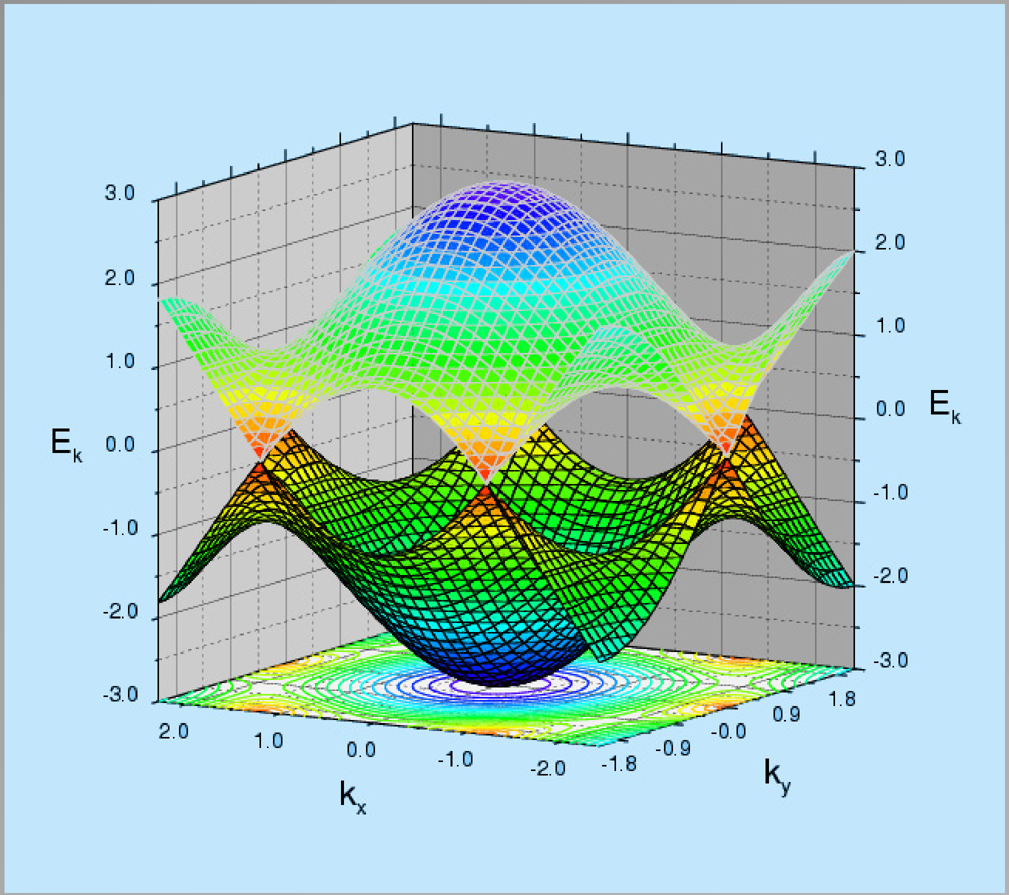
A strong paramagnetic currents appears when momentum states cross the Fermi level.

Carbon nanotubes – dispersion relation

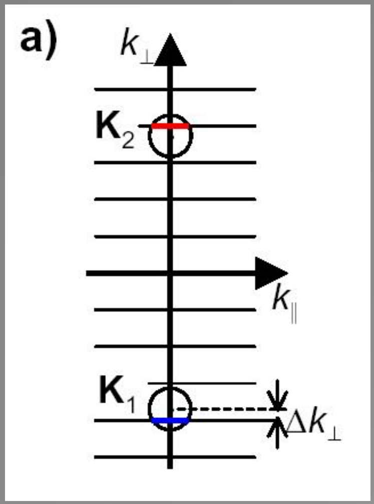
$$E(\mathbf{k}(\phi)) = \sqrt{1 + 4\cos^2(\frac{\sqrt{3}}{2}k_x(\phi)) + 4\cos(\frac{\sqrt{3}}{2}k_x(\phi))\cos(\frac{3}{2}k_x(\phi))}$$

Special features:

- Two Fermi points
- Close to conical near the Fermi points
- Deep in the Brillouin zone – nearly parabolic
- Symmetry with respect to E = 0

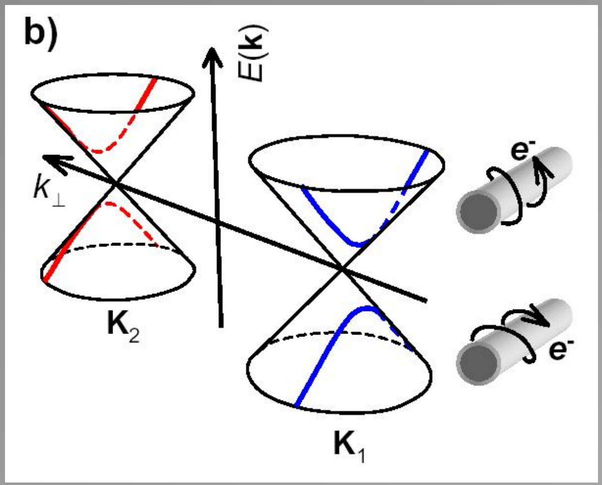


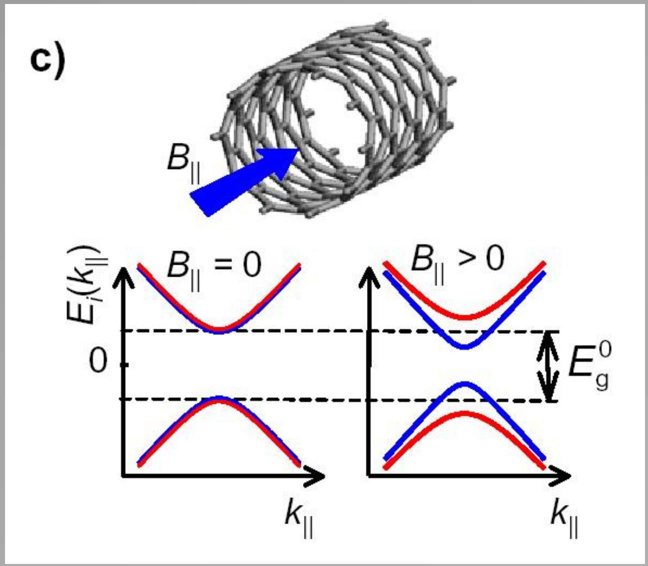
Orbital magnetic moment of an electron



Magnetic field shifts energy levels in the nanotube, changing its conduction type.

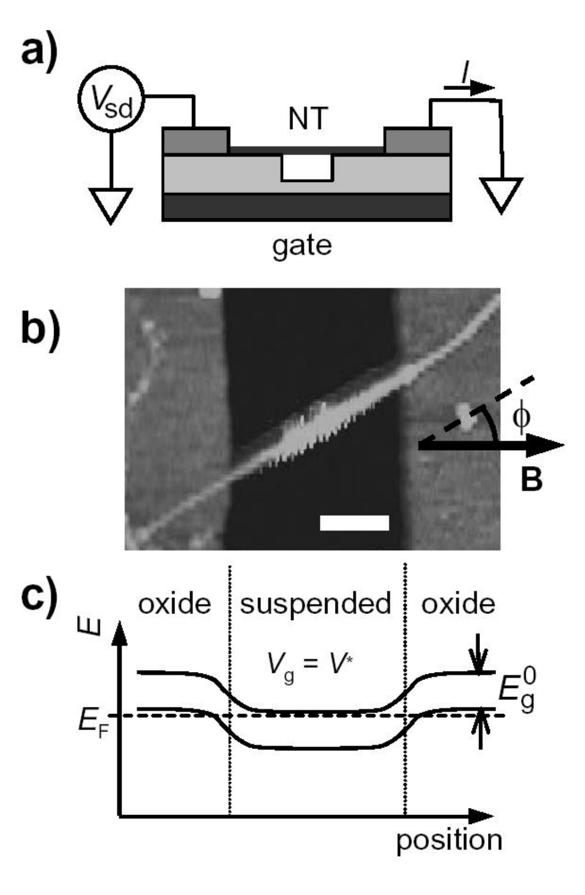
(*Ajiki, Ando J. Phys. Soc. Jpn 62 (1993) 1255*)





E.D. Minot et al., Nature 428 (2004) 536

Orbital magnetic moment of an electron



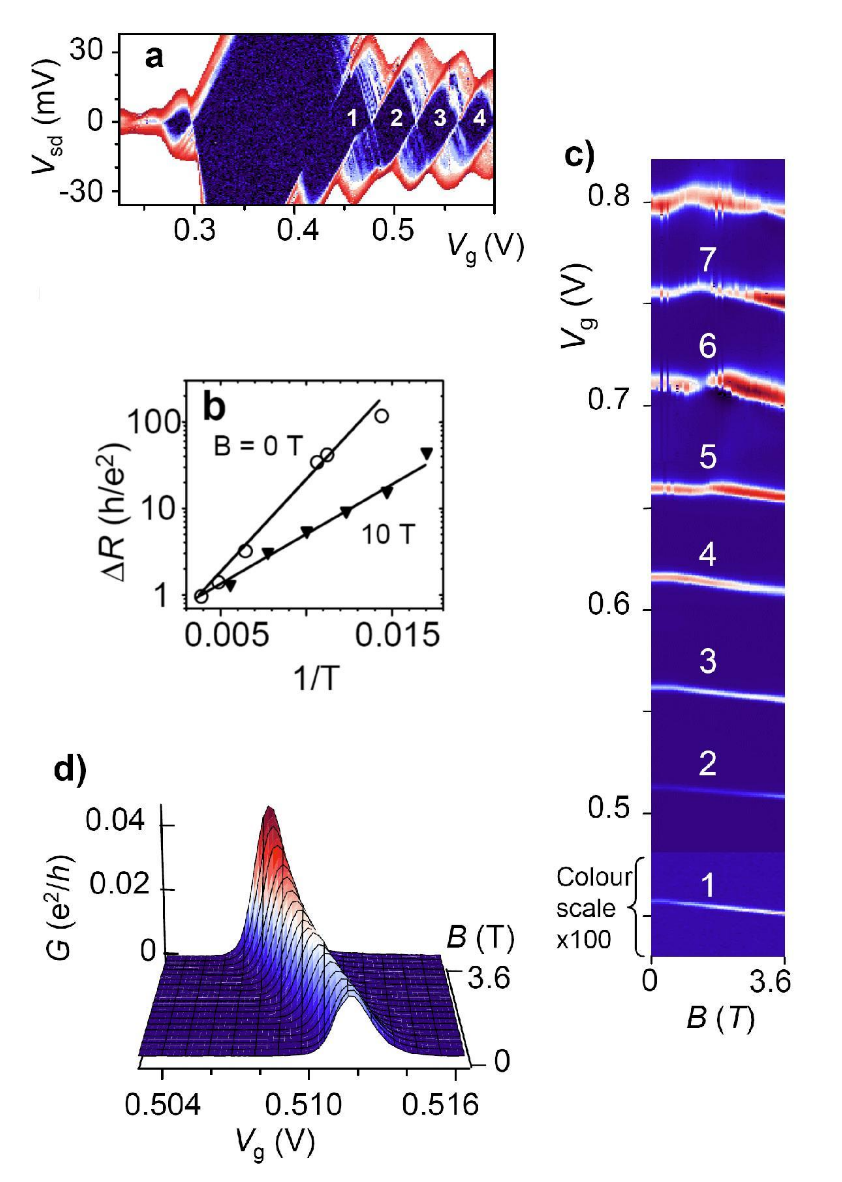
Energy shift induced by the magnetic field:

$$\Delta E \simeq \frac{\partial E}{\partial k_\perp}\Big|_{k_F} \delta k_\perp(\phi) = \pm \frac{\hbar v_F}{R}\frac{\phi}{\phi_0} = \vec{\mu}^{\,F}_{orb} \cdot \mathbf{B},$$

Thermal conductance of the nanotube in the Landauer-Büttiker formalism

$$G_{\rm act}(V^*, T) = \frac{2e^2}{h}\sum_{i=1,2}|t_i|^2 \frac{2}{\exp(E_{\rm g}^{K_i}/k_B T)+1},$$

Orbital magnetic moment of an electron



Shift in the position of conductance peaks

⟶ proof of a variation of the Fermi gap

In agreement with Ajiki & Ando hypothesis.

Full magnetic moment

Features of McEuen's approximation:

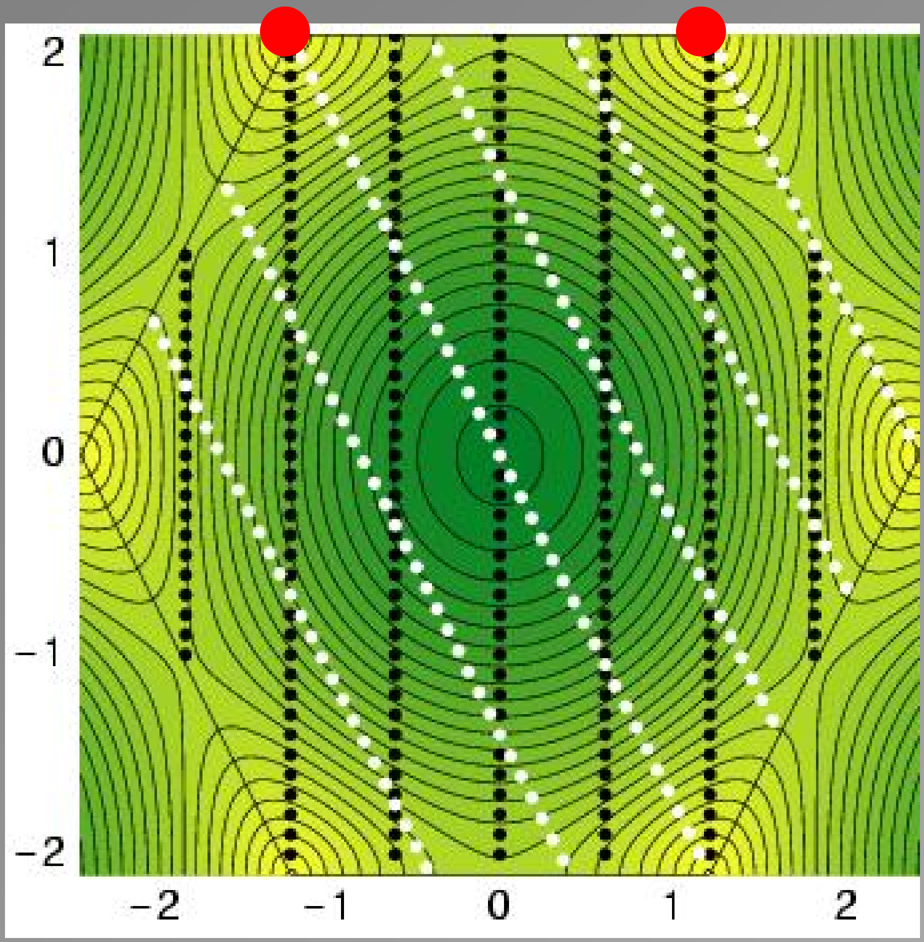
$$\Delta E \simeq \frac{\partial E}{\partial k_\perp} |_{k_F} \delta k_\perp(\phi) = \pm \frac{\hbar v_F}{R} \frac{\phi}{\phi_0} = \overrightarrow{\mu}^F_{orb} \cdot \mathbf{B},$$

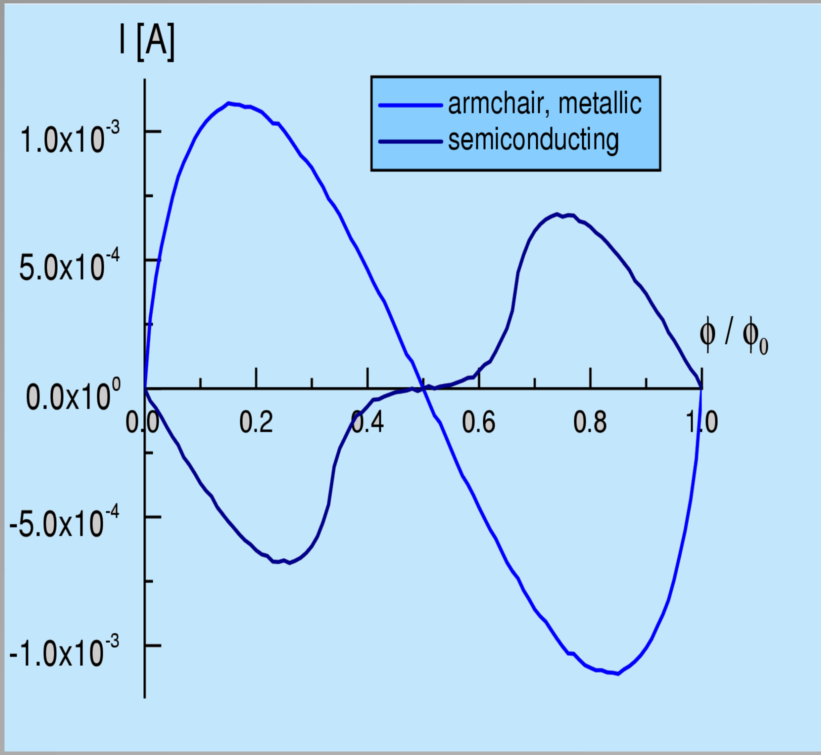
- Orbital moment independent of ϕ
- Linear increase with nanotube radius
- Neglect of temperature
- Neglect of possible doping

Full magnetic moment must contain contributions from all filled electron states:

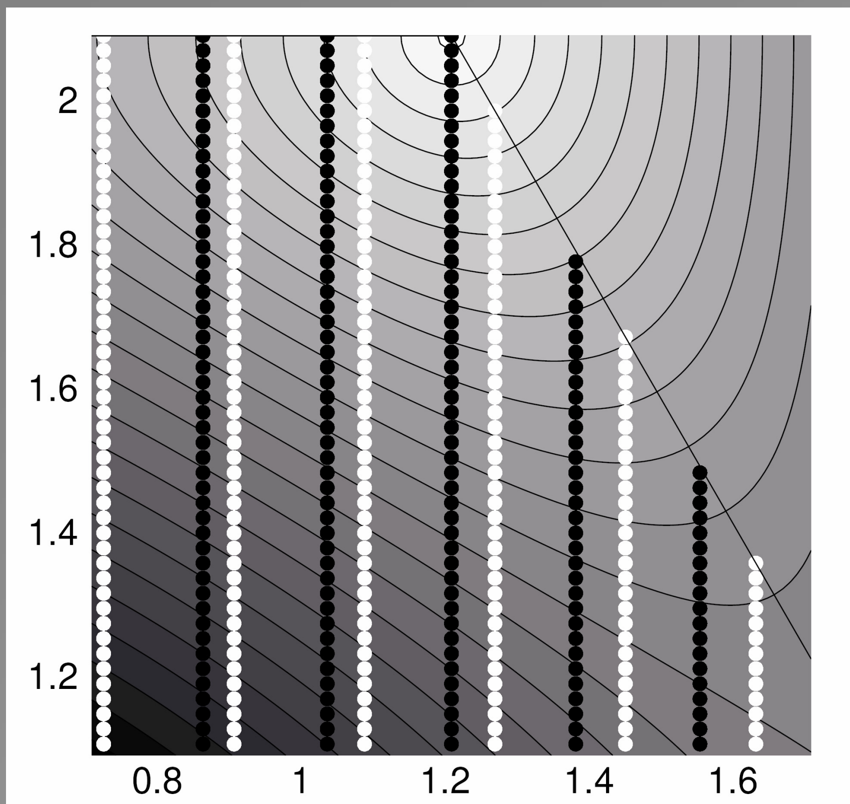
$$\mu_{orb}(\phi, T) = \pi R^2 I(\phi, T) = \pi R^2 \sum_{\mathbf{k}} \frac{1}{1 + \exp\left[(E_{\mathbf{k}}(\phi) - \mu_{chem}(\phi))/kT\right]} I_{\mathbf{k}}(\phi).$$

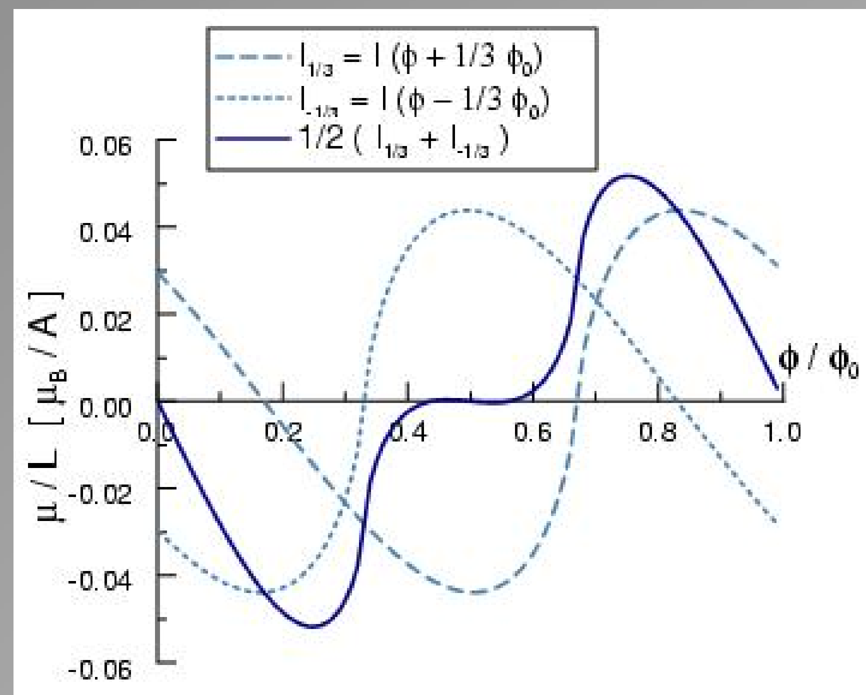
Magnetic moment in a single-wall nanotube





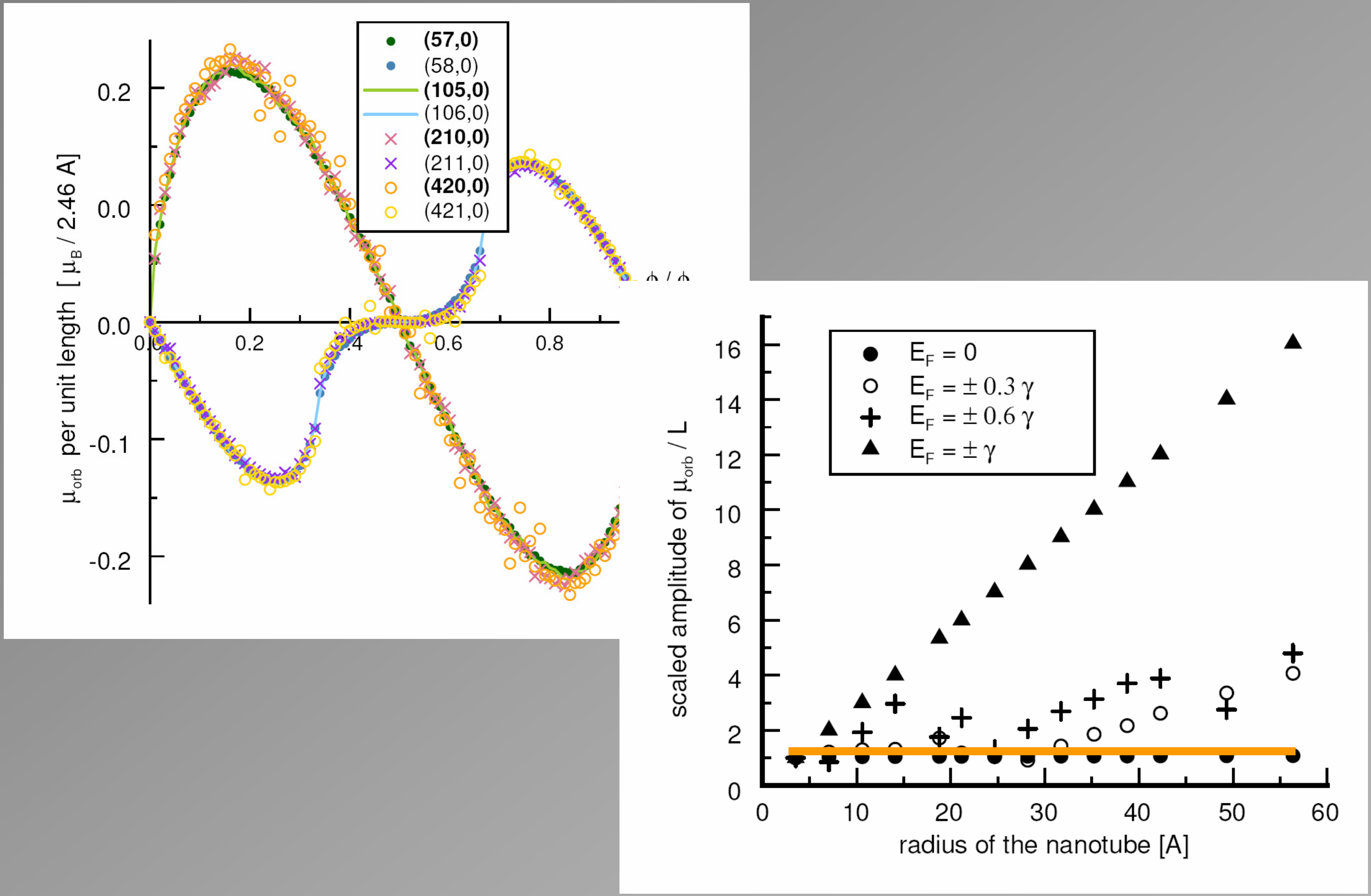
Metallic and semiconducting nanotubes





- Orbital magnetic moment in a semiconducting nanotubes is caused by two lines of momentum states, crossing the Fermi points at $-\phi_0/3$ and $+\phi_0/3$

(In?)dependence of the magnetic moment of the CN radius



Orbital magnetic moment and the Fermi surface

In metallic mesoscopic cylinders the amplitude of the overall persistent current depends strongly on the correlation of currents from the channels along the cylinder axis.

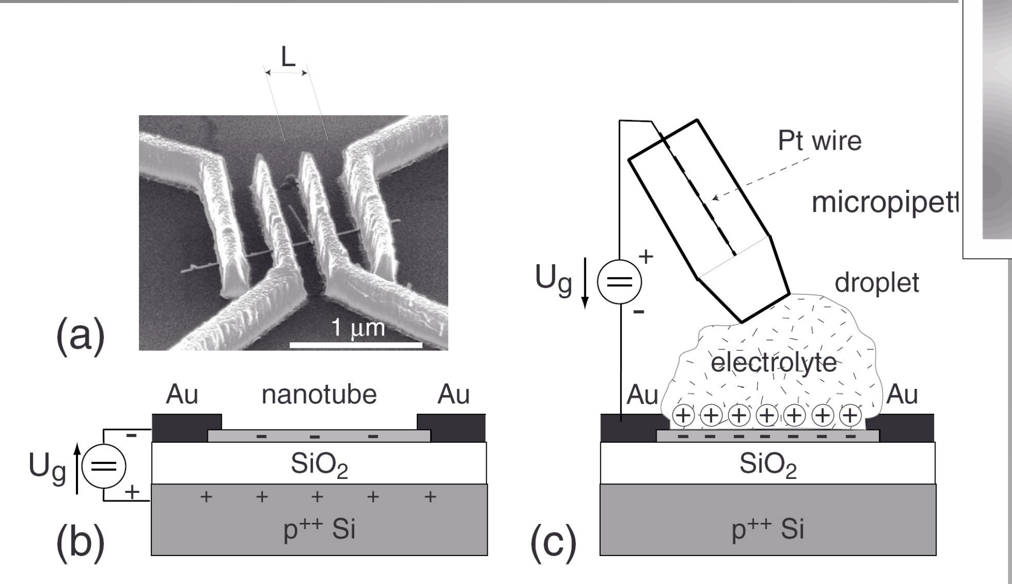
- For circular Fermi surface- weak correlation, weak current
- For flattened FS – stronger correlations, increase of the currents.
- For rectangular FS – all currents from one momentum line are correlated, the current is strongly enhanced.

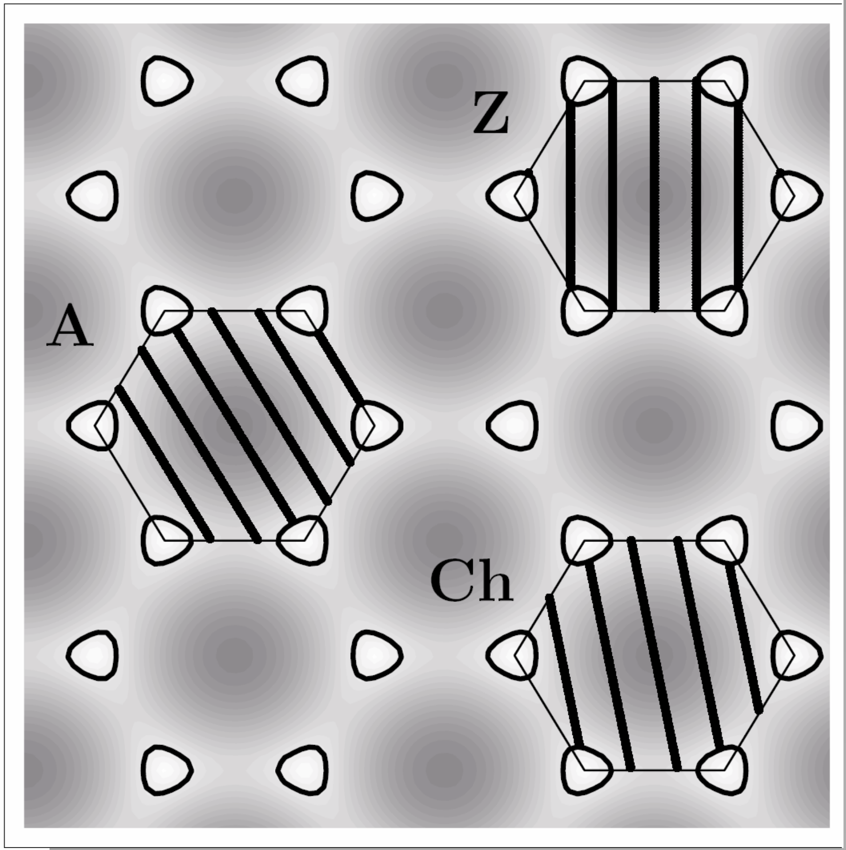
M. Stebelski et al., Eur.Phys. J. B 1 (1998) 215

Regensburg, 20.07.2005

Lowered chemical potential

M. Kruger et al.,
Appl. Phys. Lett.78 (2001) 1291



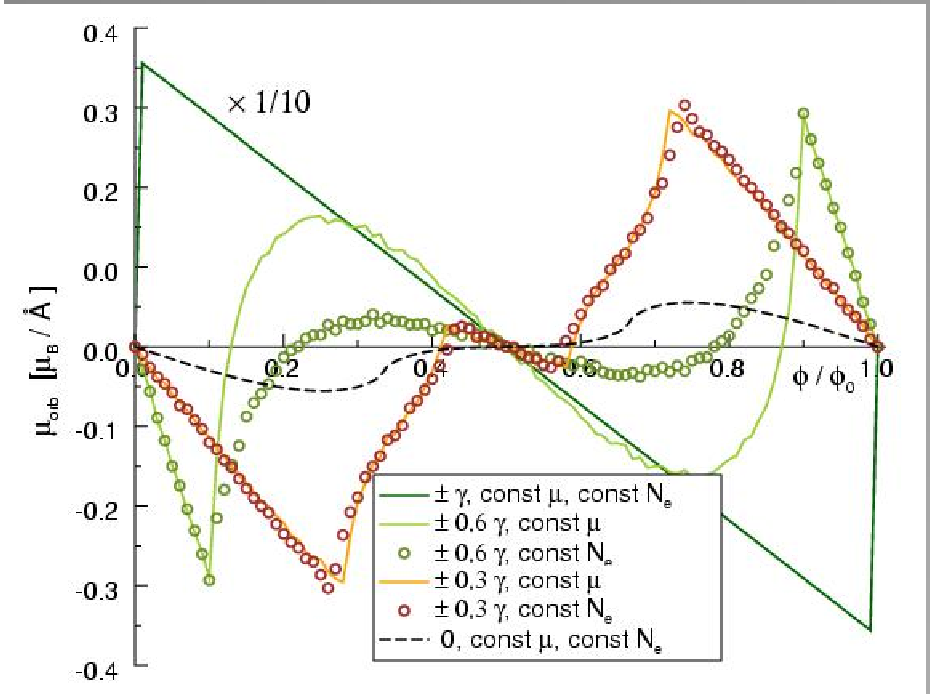


Nanotube: isolated or in a circuit

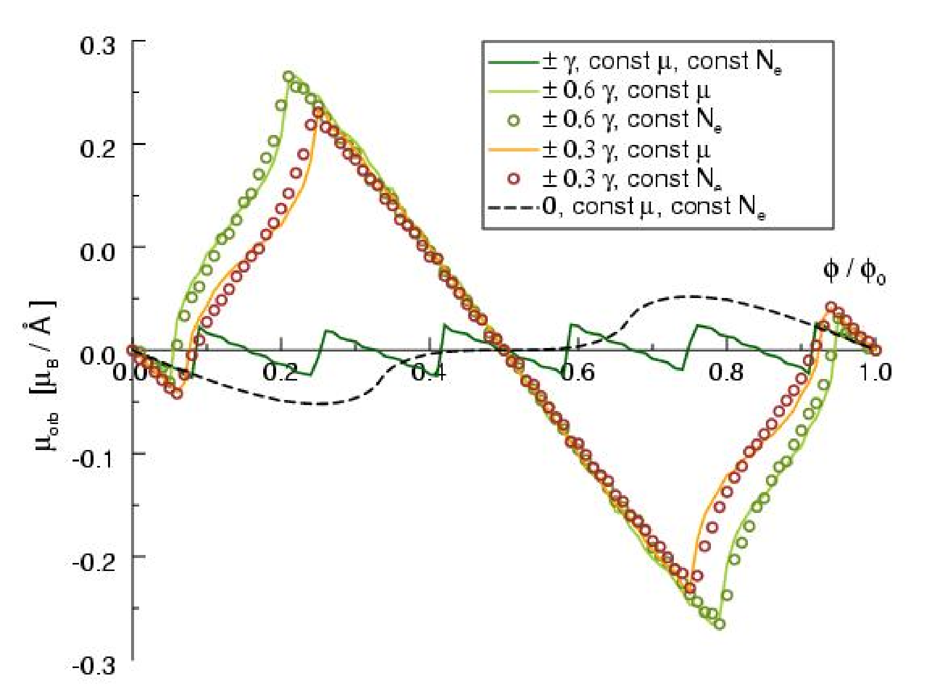
In a circuit: $\mu_{chem} = const$

Isolated: $\sum_{\mathbf{k}} f_{FD}(E(\mathbf{k}(\varphi)), \mu_{chem}, T) = N_e \rightarrow \mu_{chem}(\varphi)$

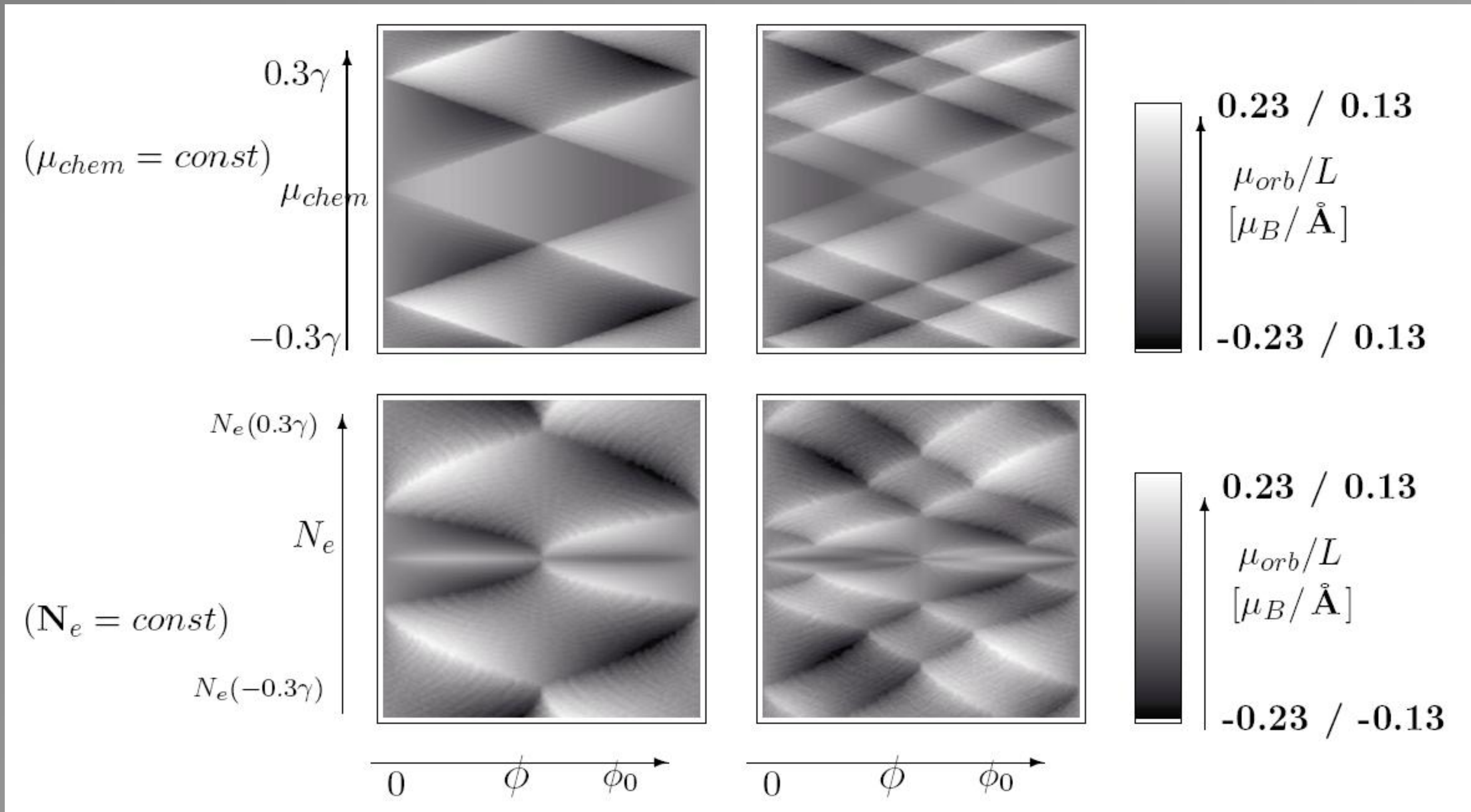
zigzag (64,0)



nearly armchair (38,36)

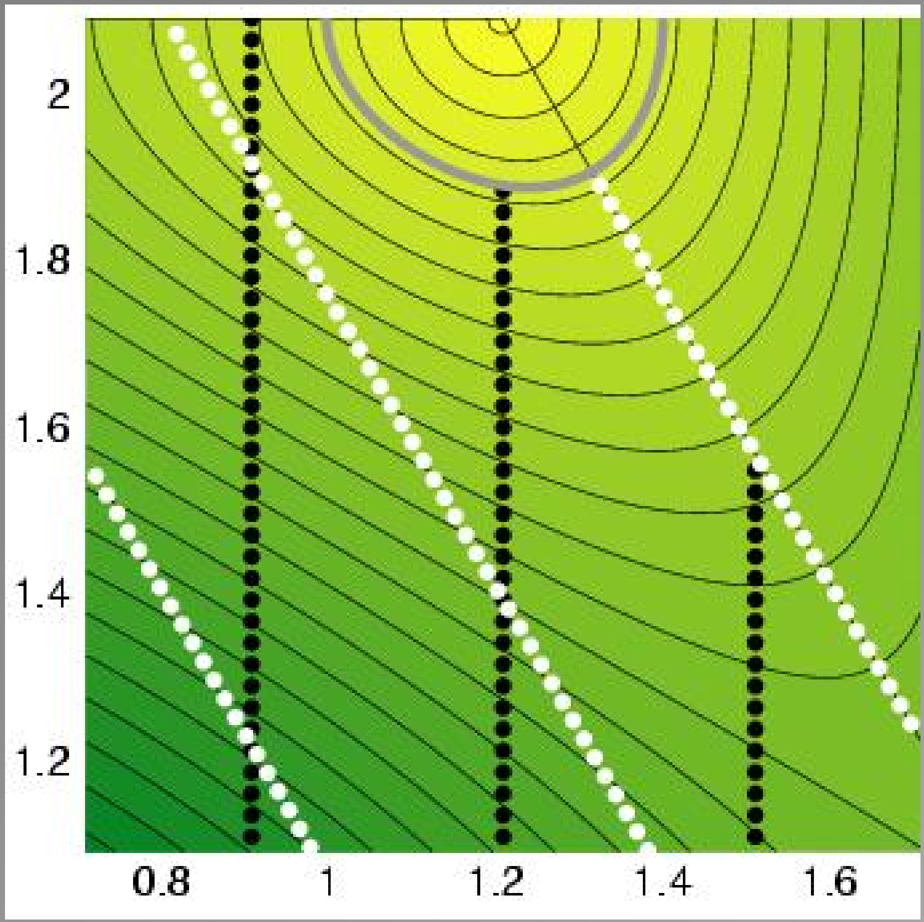


Weak doping: constant μ or constant N_e



- Top: constant μ, bottom: constant N_e
- Left: armchair (15,15), R = 10Å
- Right: chiral semiconductor (15,14), R = 10Å

Weak doping: ($\mu > -0.3\,\gamma$)



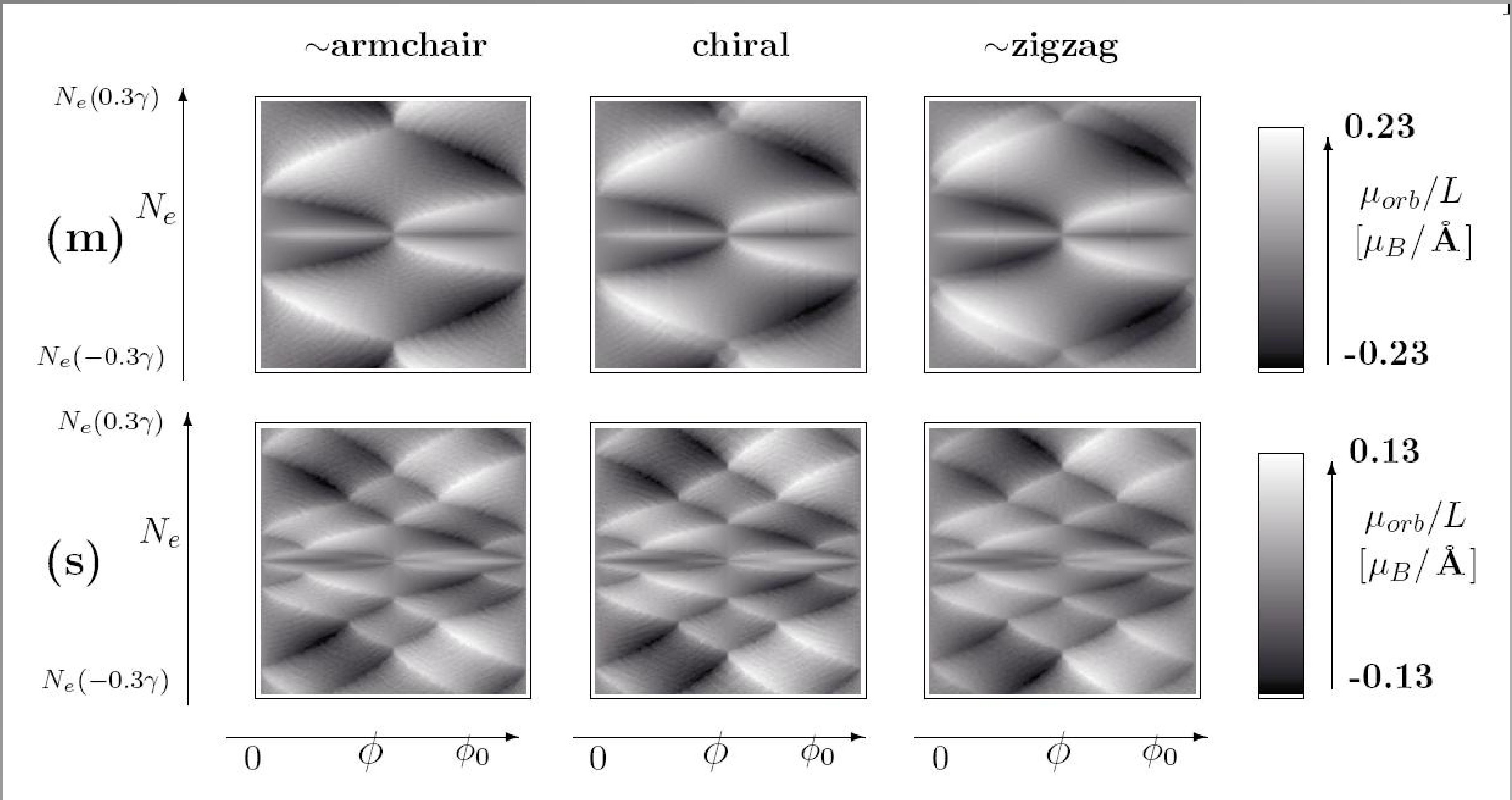
Isolated nanotube

N_e = *const*, T = 0K, R = 10 Å

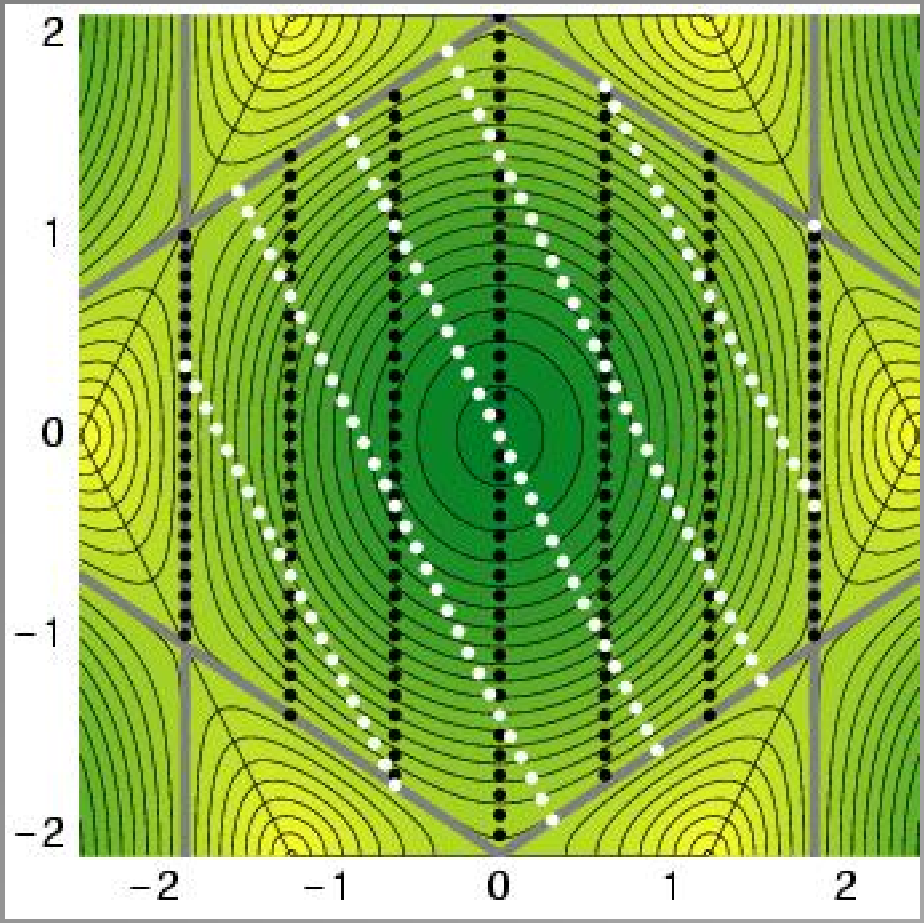
Weak doping: ($\mu > -0.3\,\gamma$)

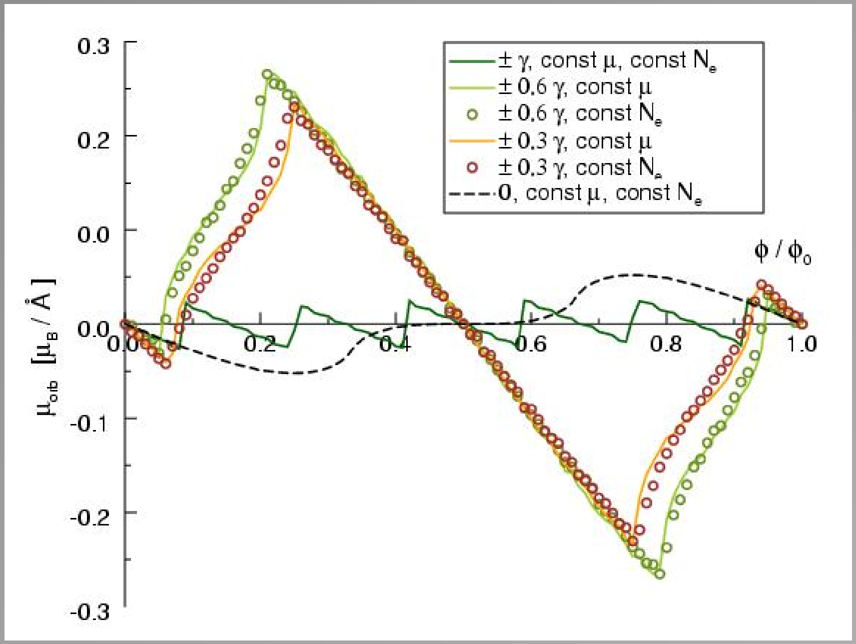
Isolated nanotube

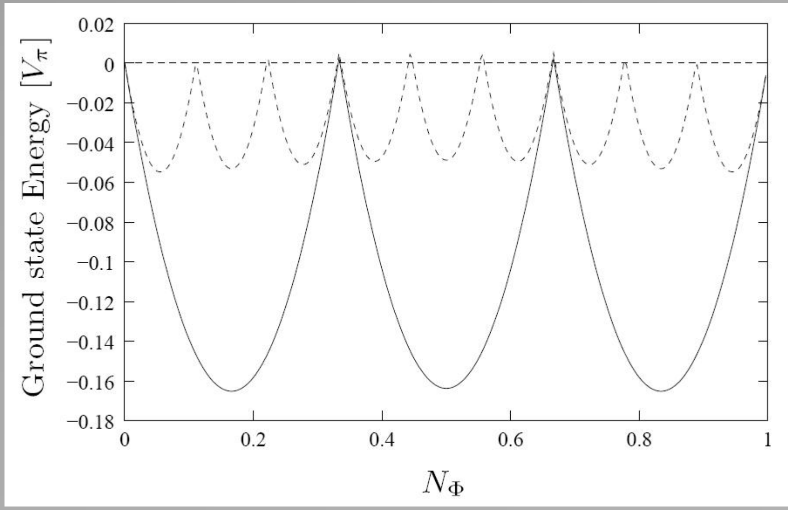
N_e = *const*, T = 0K, R = 10 Å



Special case: $\mu > -\gamma$

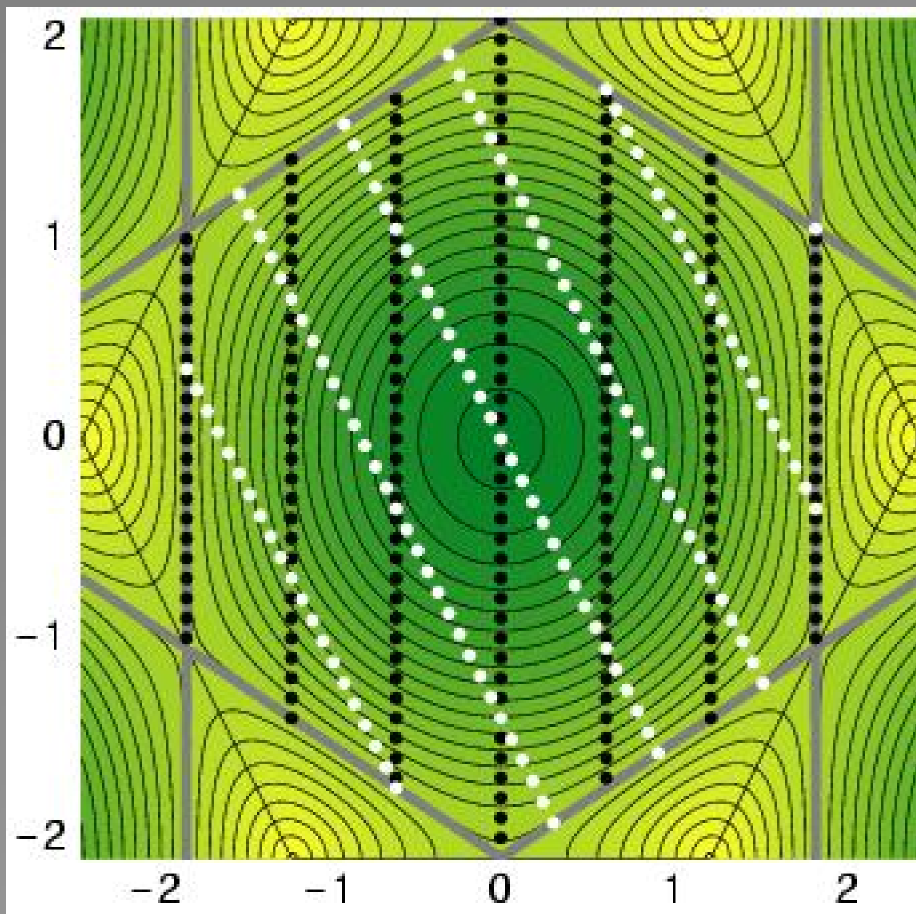


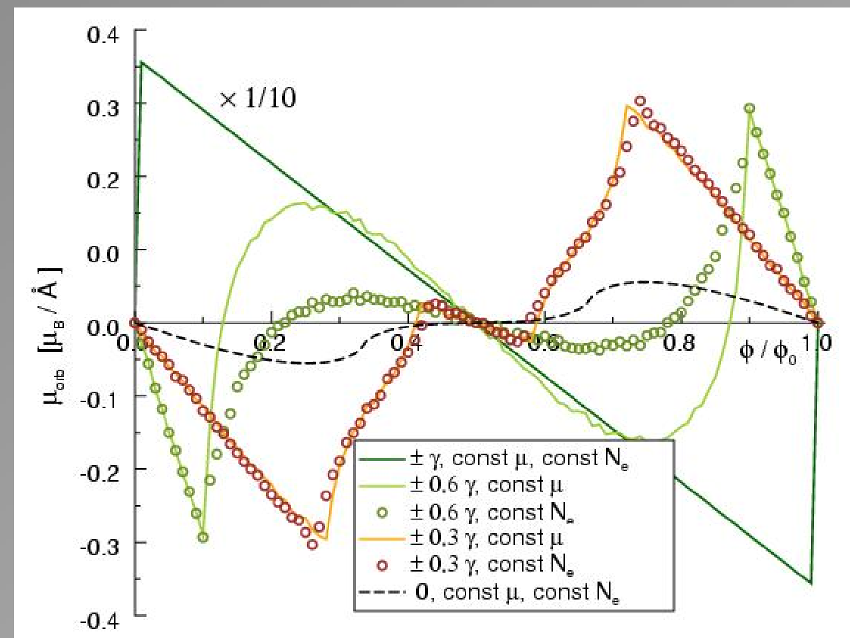


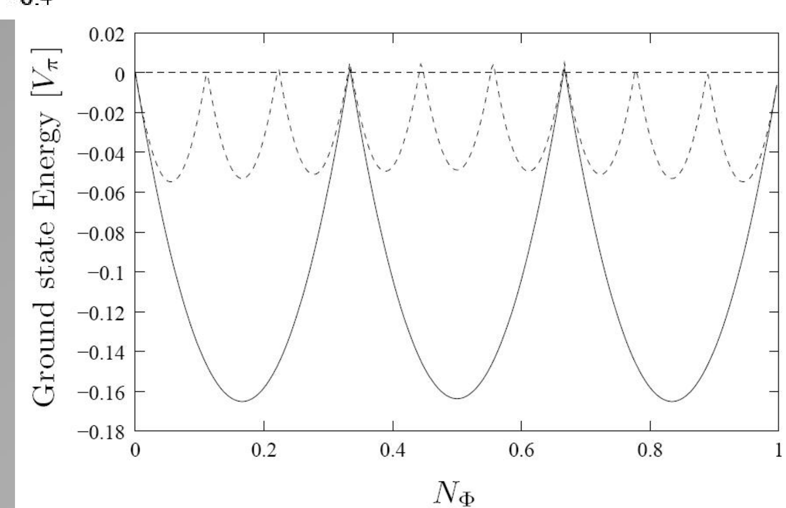


K. Sasaki et al., cond-mat/0407539

Special case: $\mu > -\gamma$

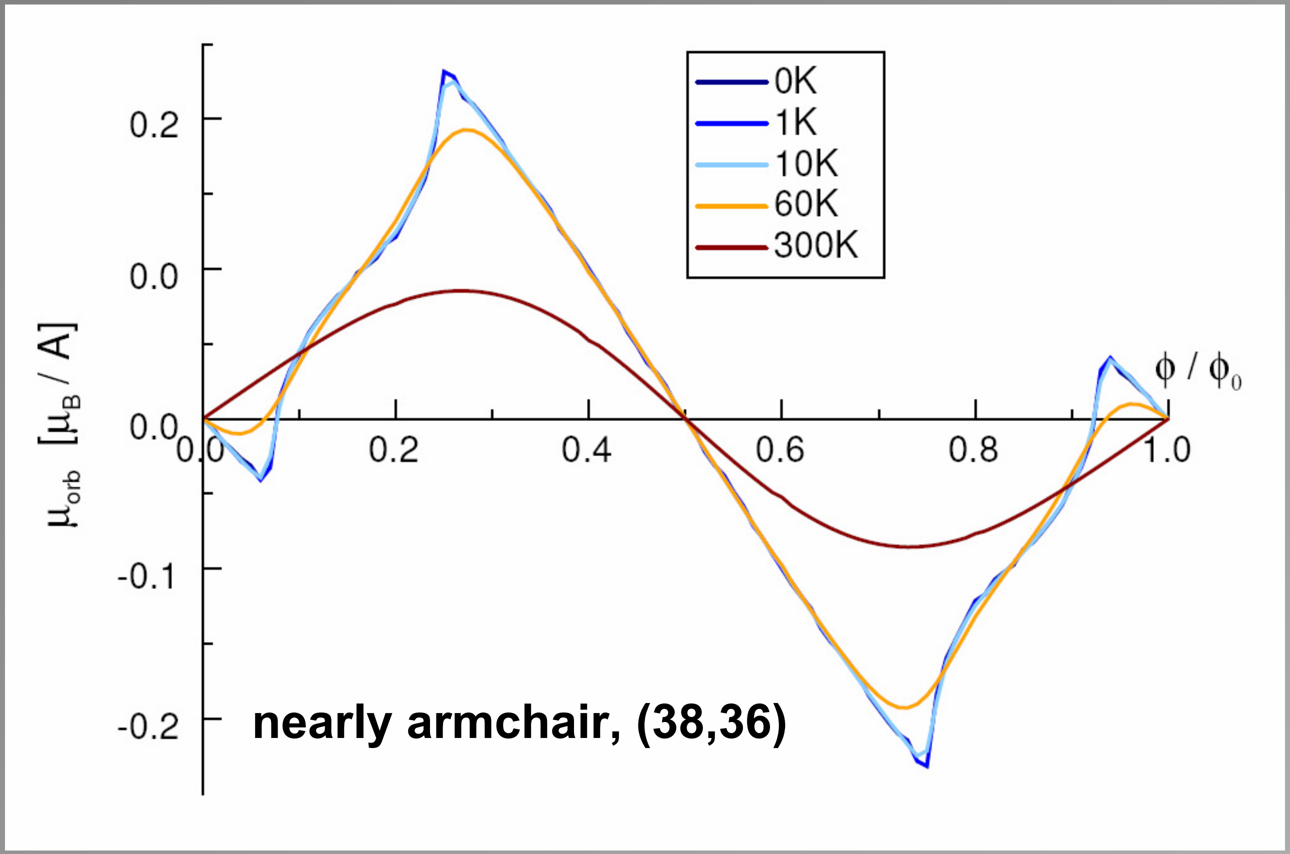






K. Sasaki et al., cond-mat/0407539

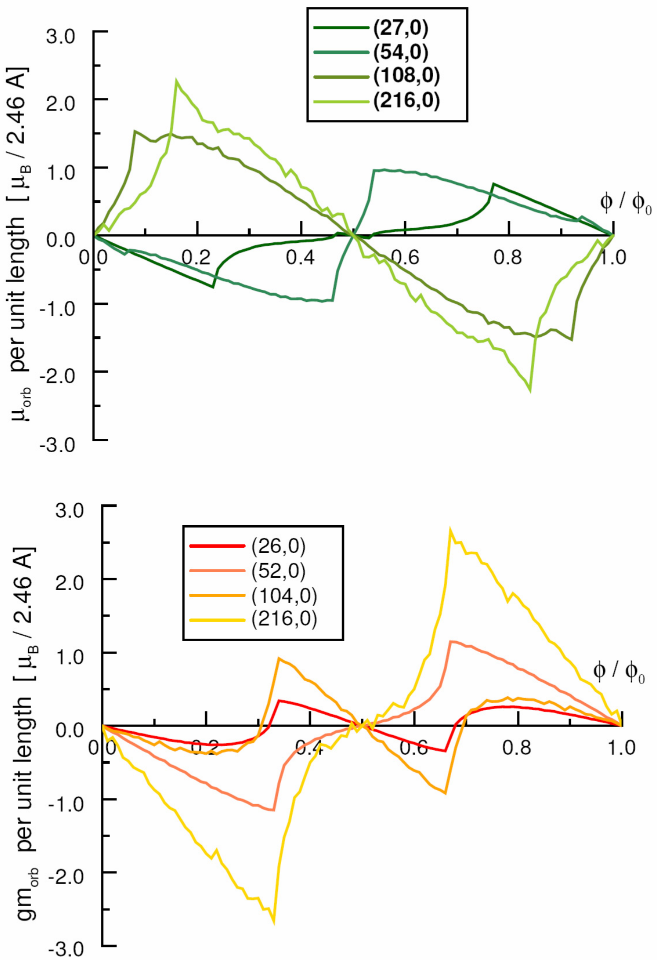
Dependence of the magnetic moment on temperature



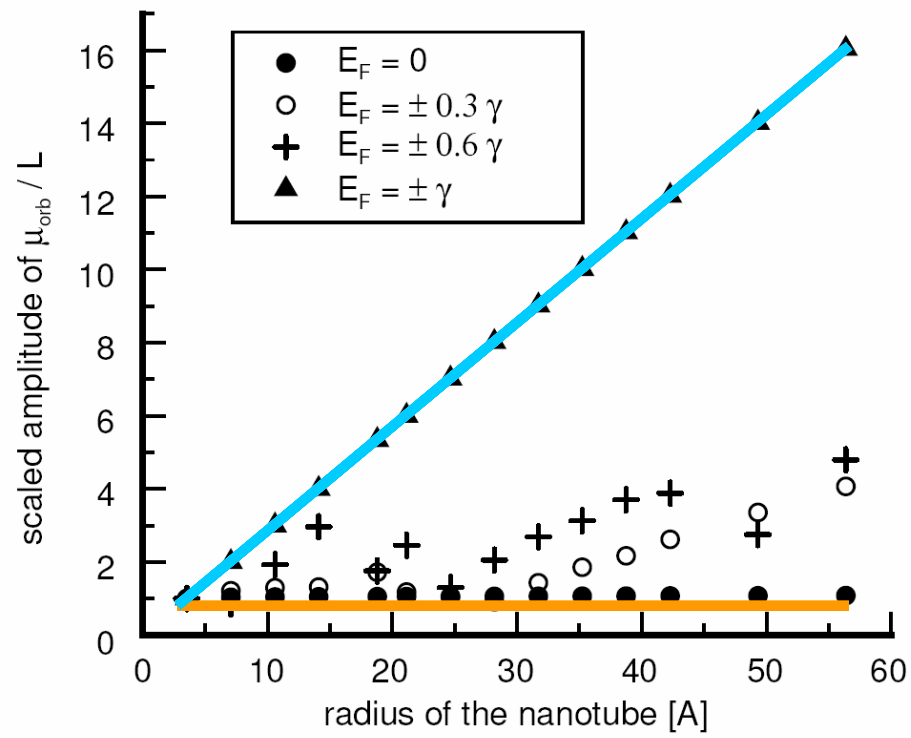
- Main effect – decrease in the amplitude and reduction of sharp features

Dependence on radius of μ_{orb} in doped nanotubes

metallic, zigzag



semiconducting, zigzag

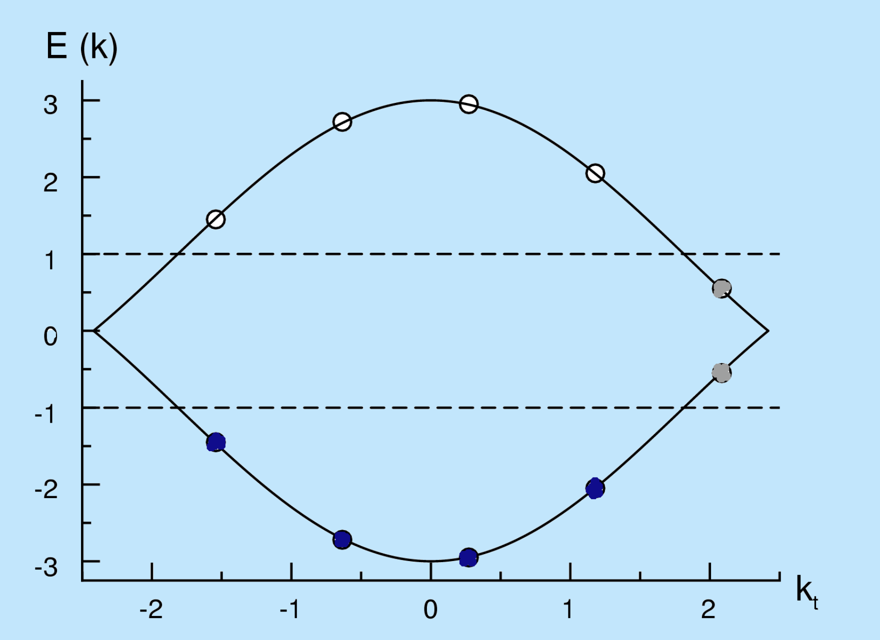


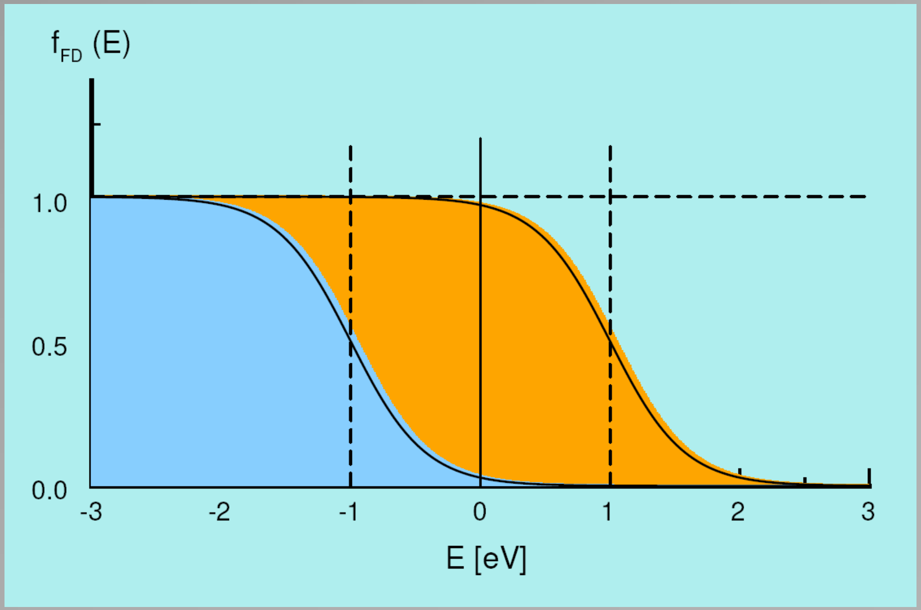
Electron-hole symmetry

A combination of:

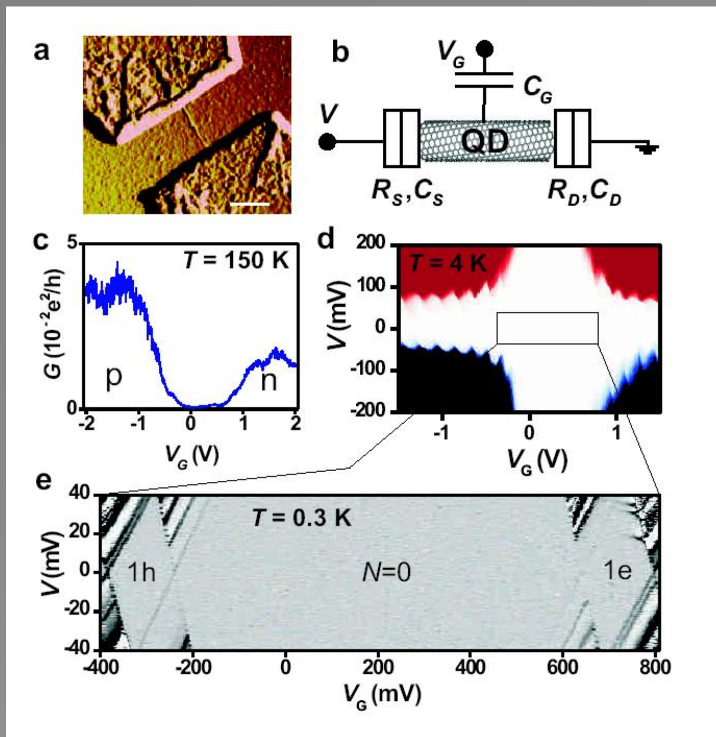
- electron-hole symmetry of graphene’s dispersion relation
- Fermi-Dirac function symmetry with respect to the chemical potential

leads to electron-hole symmetry both in persistent and transport currents.

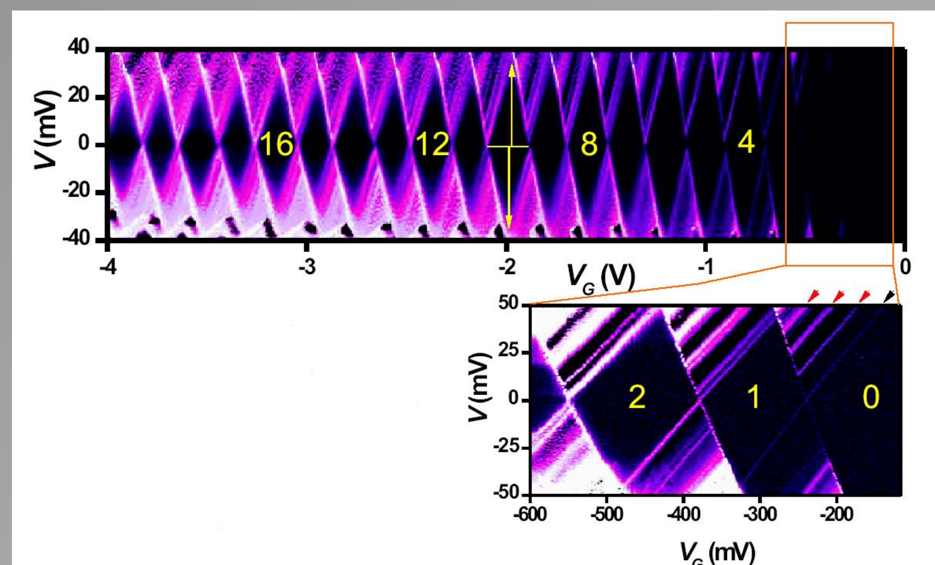




Electron-hole symmetry, an experiment

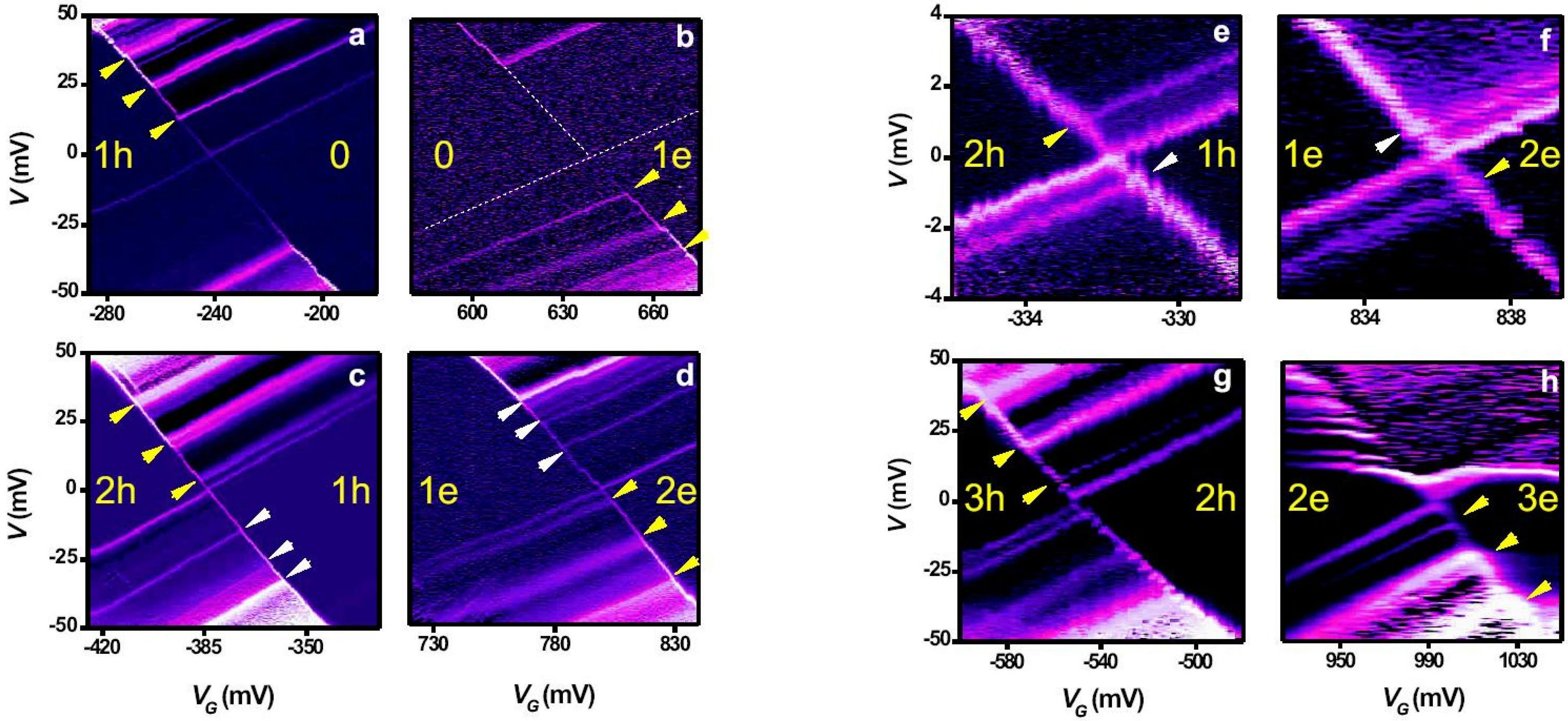


Semiconducting nanotube quantum dot, chemical potential controlled by the gate voltage.



P. Jarillo-Herrero et al.., Nature 429 (2004), 389

Electron-hole symmetry, an experiment



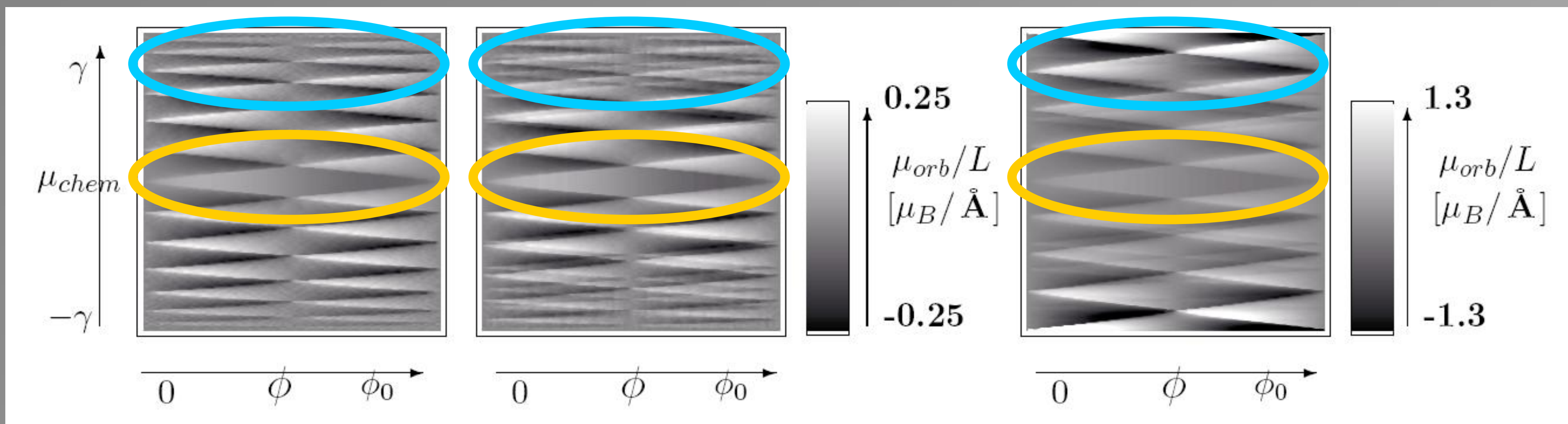
Each conduction line for electrons corresponds to its analogue for holes.

Full symmetry of the Coulomb blockade pattern.

Strong doping

Metallic nanotubes

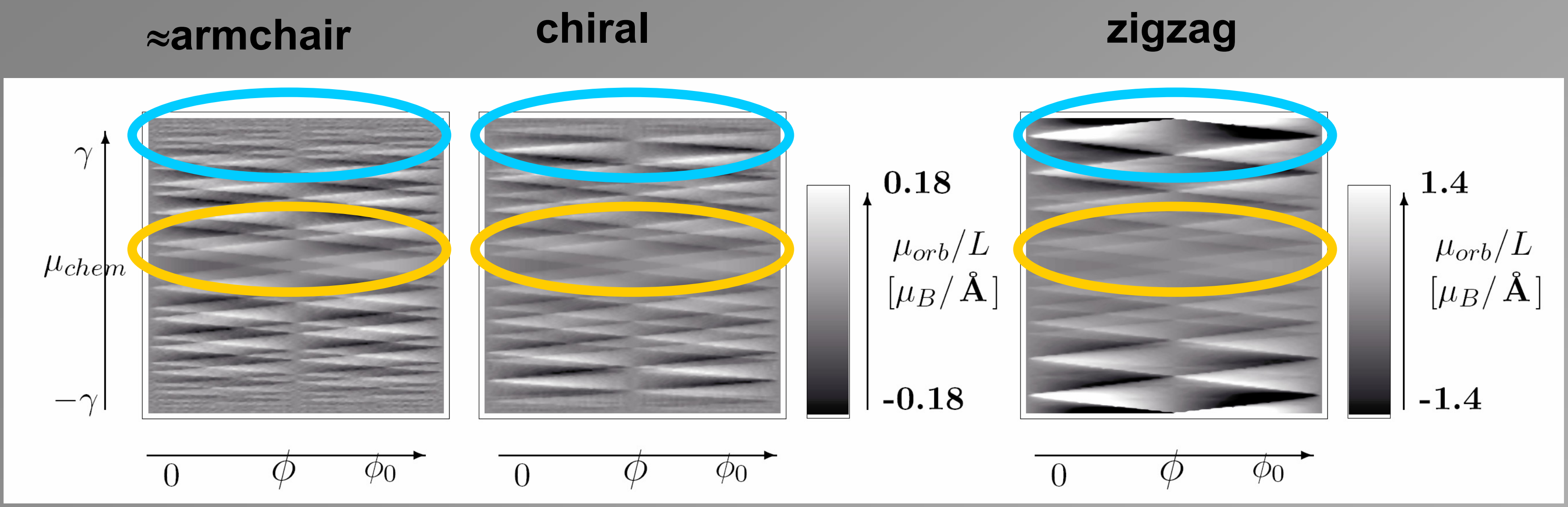
armchair **chiral** **zigzag**



- ➔ ϕ dependence similar for small doping, distinct differences for large doping
- ➔ Electron-hole symmetry
- ➔ Extraordinary increase of the magnetic moment in strongly doped zigzags

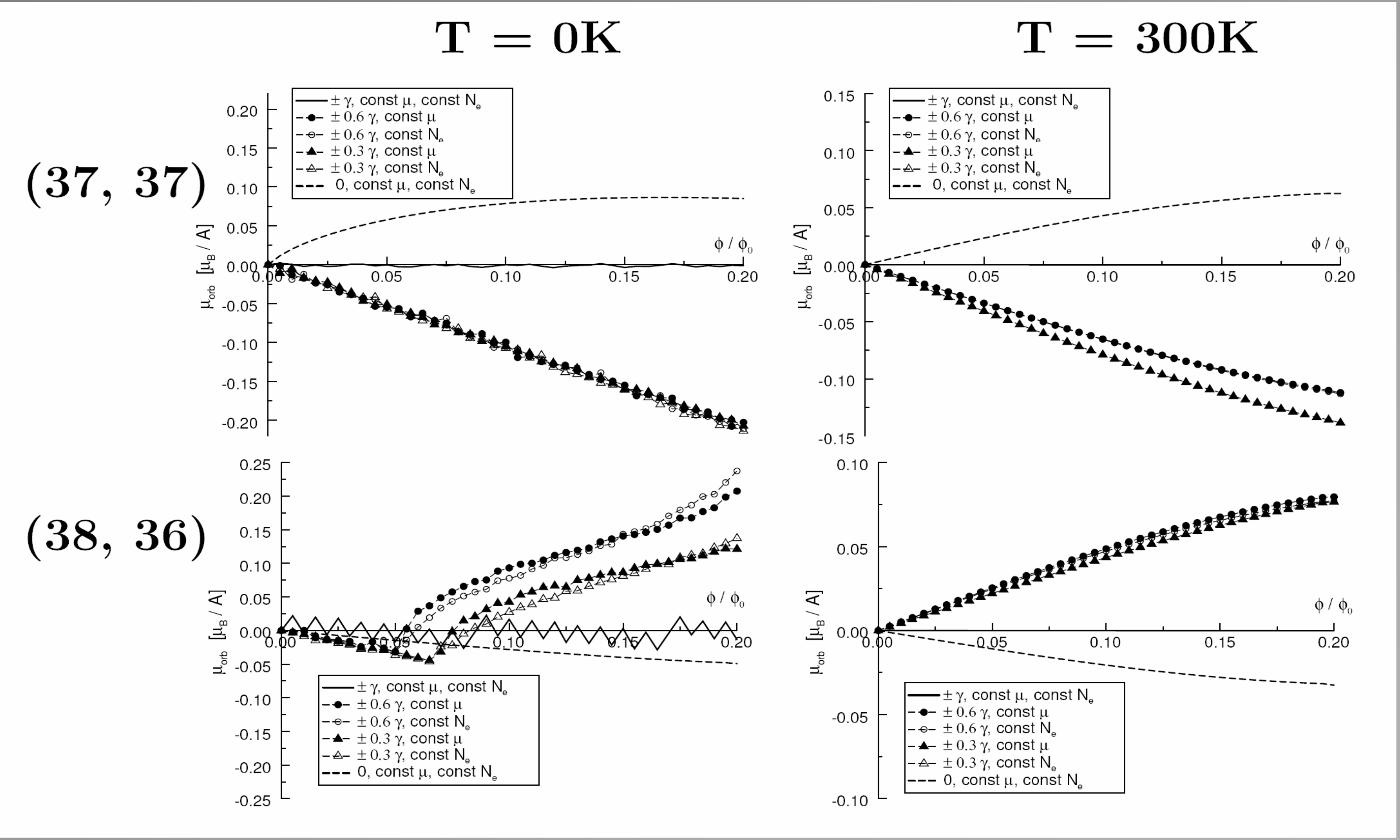
Strong doping

Semiconducting CN



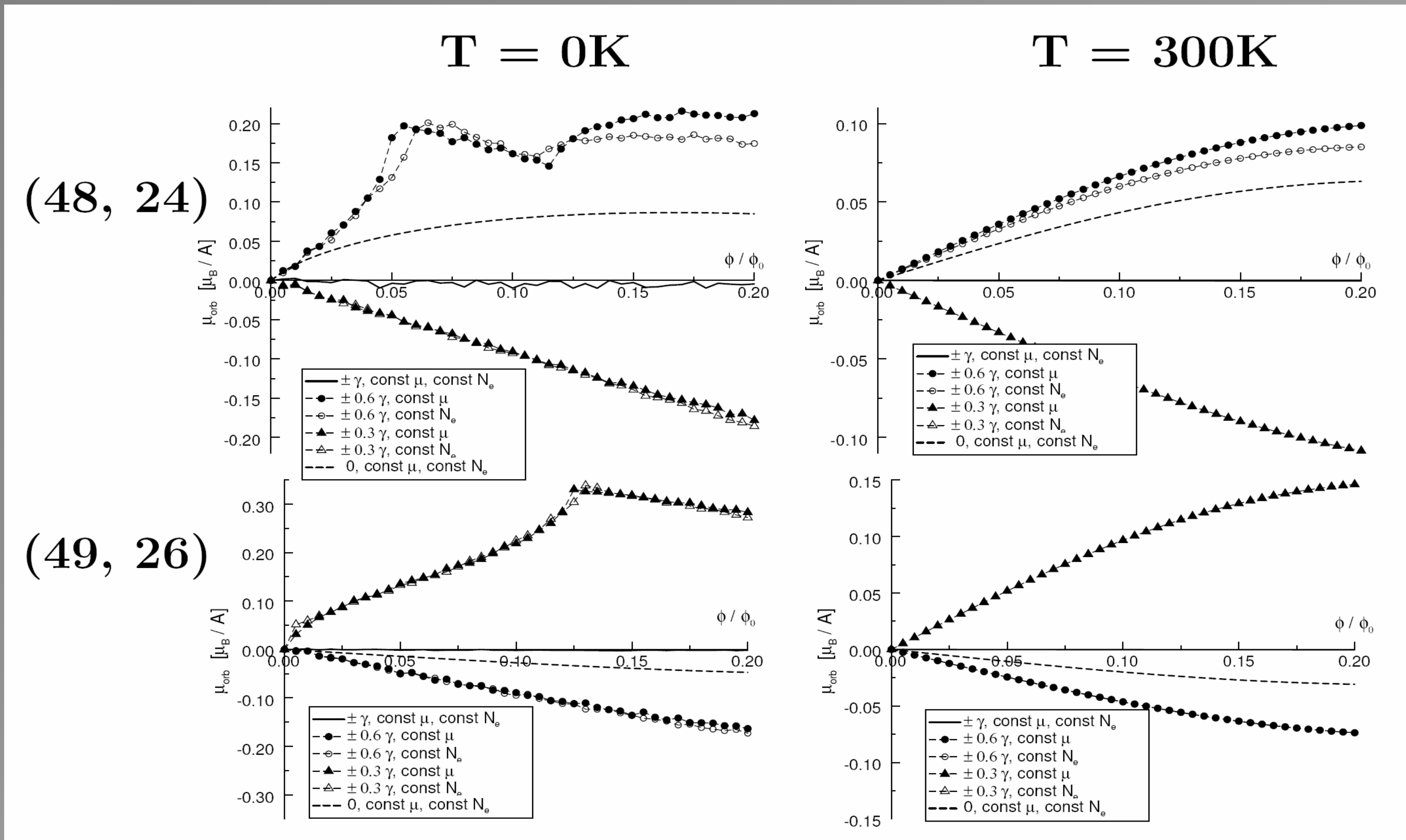
- ➔ ϕ dependence similar for small doping, distinct differences for large doping
- ➔ Electron-hole symmetry
- ➔ Extraordinary increase of the magnetic moment in strongly doped zigzags

Weak magnetic fields - armchair



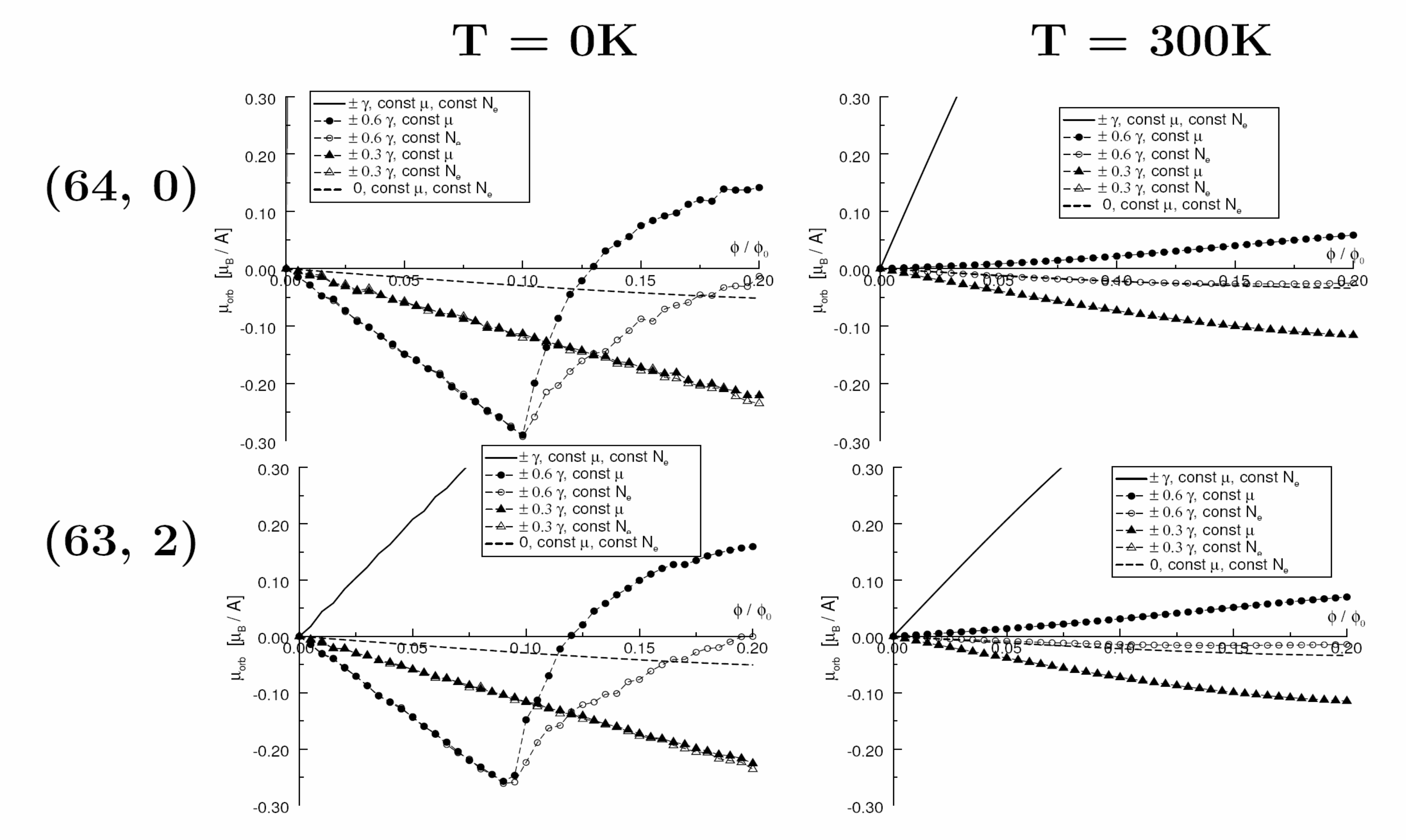
Regensburg, 20.07.2005

Weak magnetic fields - chiral



Regensburg, 20.07.2005

Weak magnetic fields - zigzags



Orbital magnetic moment for B < 20T

Nanotube in a circuit,

μ = const, T = 0 K, R = 25 Å, L = 0.1μm

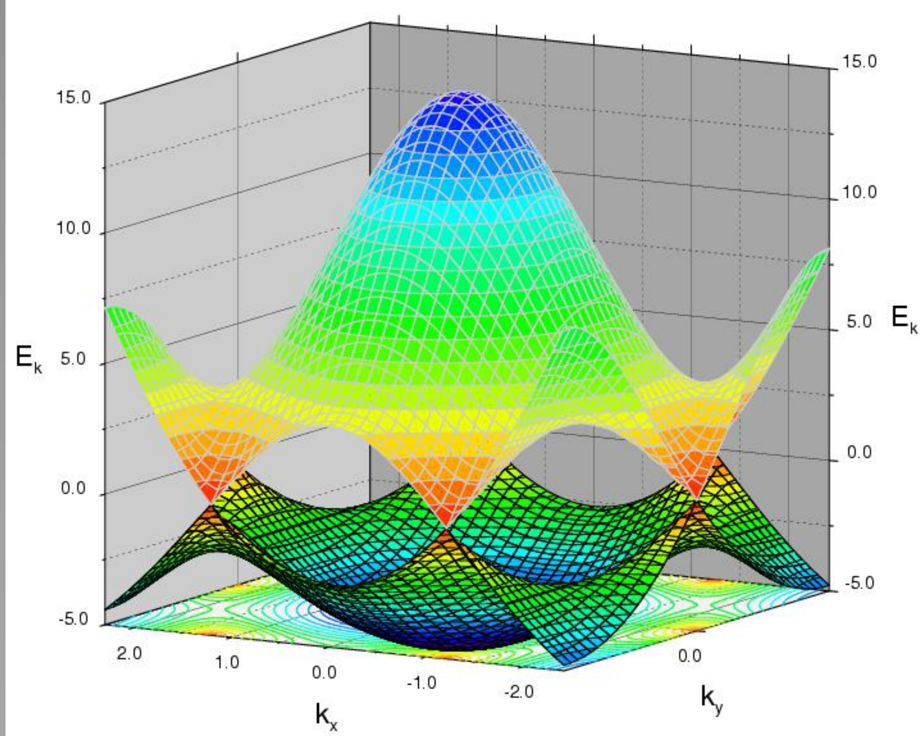
	$E_F = 0$	$E_F = \pm 0.3\gamma$	$E_F = \pm 0.6\gamma$	$E_F = \pm\gamma$
armchair (37,37)	78.7 *(42.9)*	-100 *(-78.9)*	-99.5 *(-65.1)*	≤ 3 *(≤ 1)*
chiral S (38,36)	-28.2 *(-20.5)*	42.6 *(43.5)*	93.2 *(48.6)*	-26.4 ($\leq$ *1*)
chiral M (48,24)	78.7 *(43.3)*	-90.6 *(63.9)*	161.6 *(66.4)*	-9.7 ($\leq$ *2*)
chiral S (49,23)	-27.5 *(-20)*	218.8 *(96.7)*	-89.1 *(-46.3)*	≤ 2 ($\leq$ *2*)
chiral S (63,2)	-29.3 *(-21.8)*	-116.9 *(-72.7)*	-148.1 *(31.1)*	399.2 *(389)*
zigzag M (63,0)	80.2 *(44.1)*	-62.5 *(-28.7)*	28.7 *(-63.1)*	-714.7 *(-523)*
zigzag S (64,0)	-29.8 *(-21.9)*	-113.3 *(-73.2)*	-290 *(21.8)*	3559, at $B \ll 1$T *(818.2)*

Carbon nanotubes – asymmetric dispersion relation

Special features:

- Two Fermi points
- Close to conical near the Fermi points
- Deep in the Brillouin zone – nearly parabolic

$$E_{\mathbf{k}(\phi)} = \frac{\epsilon_{2p} \pm \gamma\, w_{\mathbf{k}(\phi)}}{1 \mp s\, w_{\mathbf{k}(\phi)}}$$

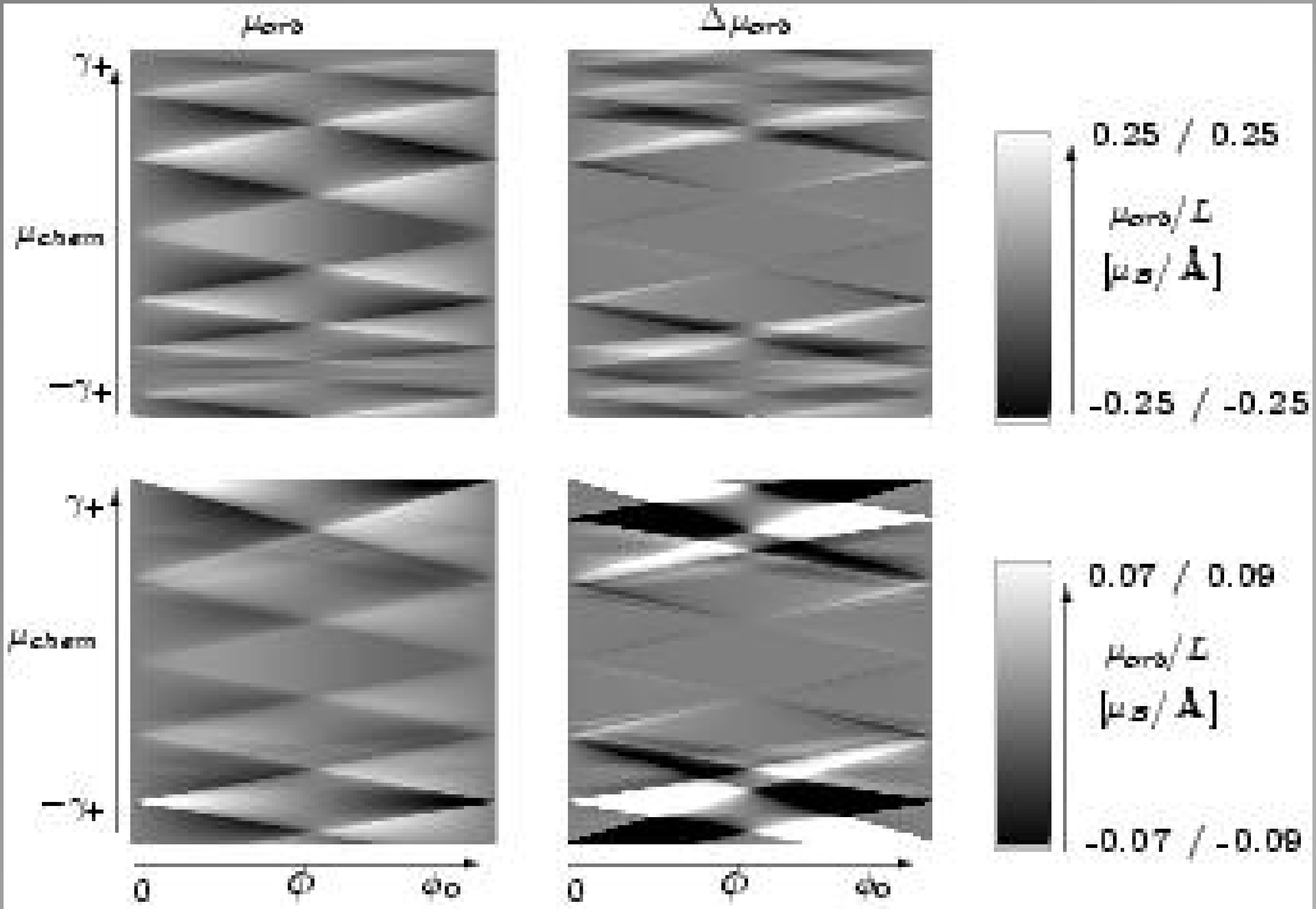


s ~ 0.13 - overlap between π orbitals at neighbouring sites in graphene

Asymmetric dispersion, orbital magnetic moment for hole- and electron doping

Armchair

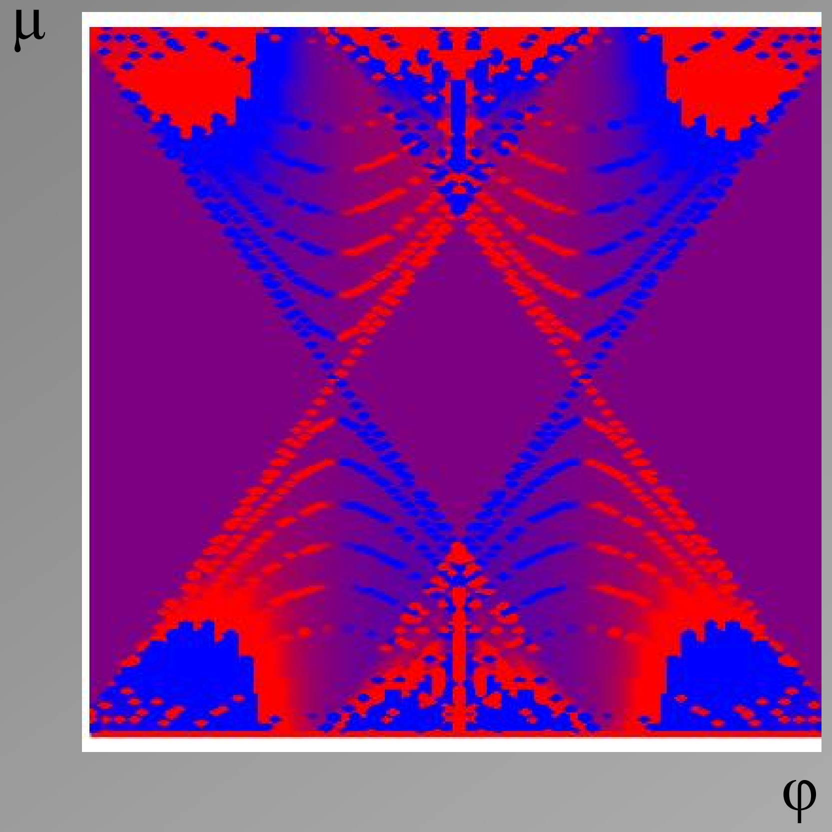
Zigzag



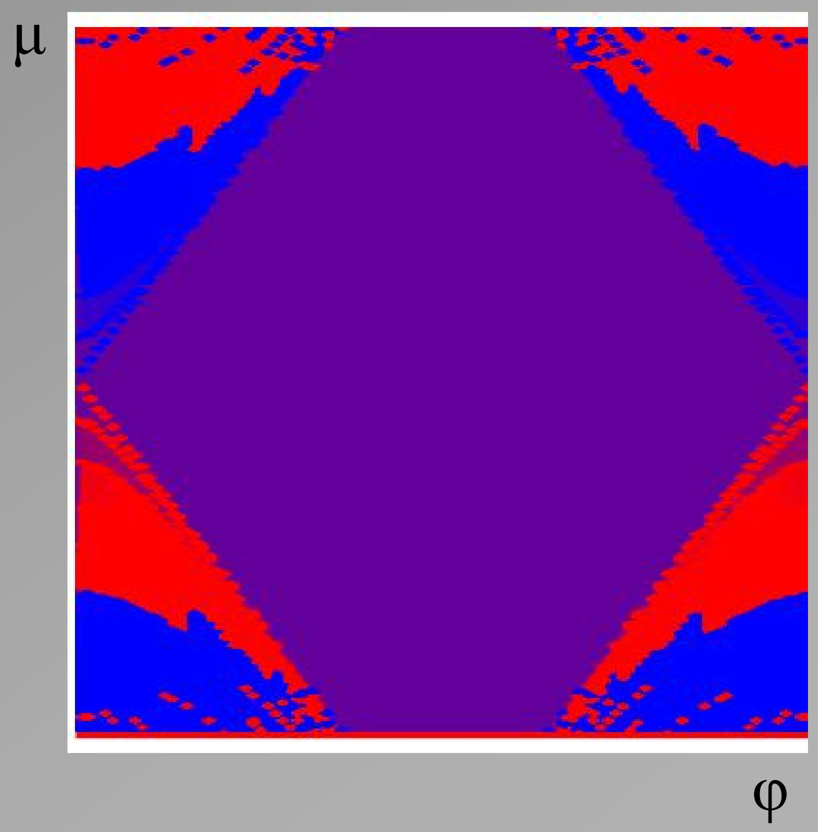
Asymmetric dispersion, orbital magnetic moment for holes and electrons

Difference between hole and electron magnetic moments for nanotubes from the Jarillo-Herrero experiment, R=2.6nm, 35 holes to 35 excess electrons

(20,19 semiconducting)



(20,20) metallic



Asymmetric dispersion, orbital magnetic moment for B < 20T

Nanotube in a circuit,

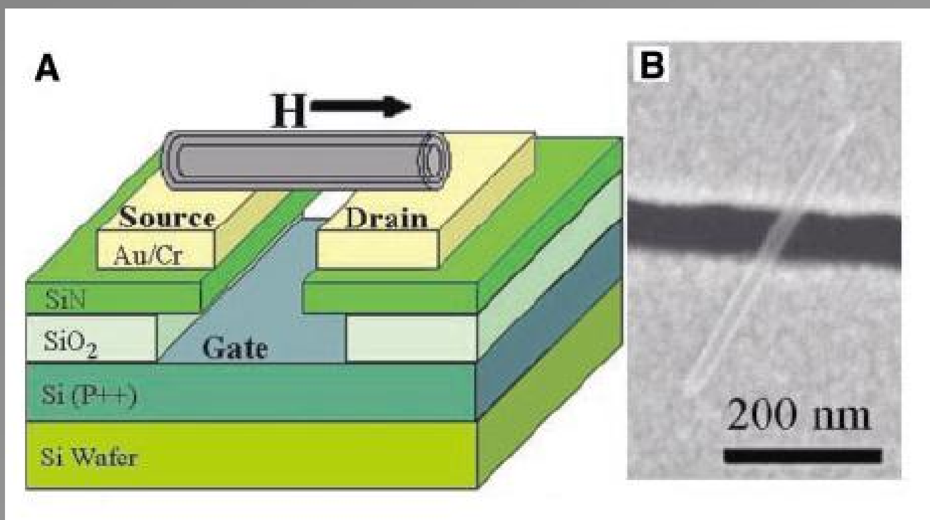
μ = const, T = 0 K, R = 25 Å,

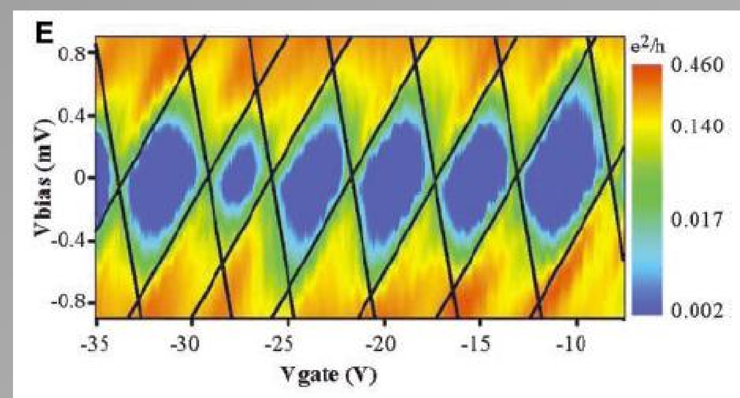
L = 0.1μm

μ_{chem}	0	$-0.3\gamma_-(+0.3\gamma_+)$	$-0.6\gamma_-(+0.6\gamma_+)$	$-\gamma_-(+\gamma_+)$
armchair (37,37)	26	5.1 *(48)*	46 *(122)*	≤ 1 ($\leq$ *1*)
chiral S (38,36)	-9	-26 *(-20)*	-39 *(-35)*	-8 *(9)*
chiral M (48,24)	26	19 *(23)*	-34 *(-25)*	-3 *(-4)*
chiral S (49,23)	-9	-46 *(-21)*	-23 *(37)*	≤ 1 ($\leq$ *1*)
chiral S (63,2)	-9.7	29 *(59)*	-49 *(12)*	**117** ***(151)***
zigzag M (63,0)	26	67 *(19)*	37 *(-96)*	**-210** ***(-270)***
zigzag S (64,0)	-9.8	29.6 *(59.6)*	-49 *(16)*	**1060** ***(1370)***, at $B \ll 1$T

Aharonov-Bohm effect in multiwall nanotubes

- Magnetic field necessary to obtain ϕ_0 in a single-wall nanotube (R ≅ 2.5 nm) ⟶ **B = 210 T** !
- This difficulty can be circumvented by the use of multiwall nanotubes (R ≅15 nm, **B(ϕ_0) = 6 T**)



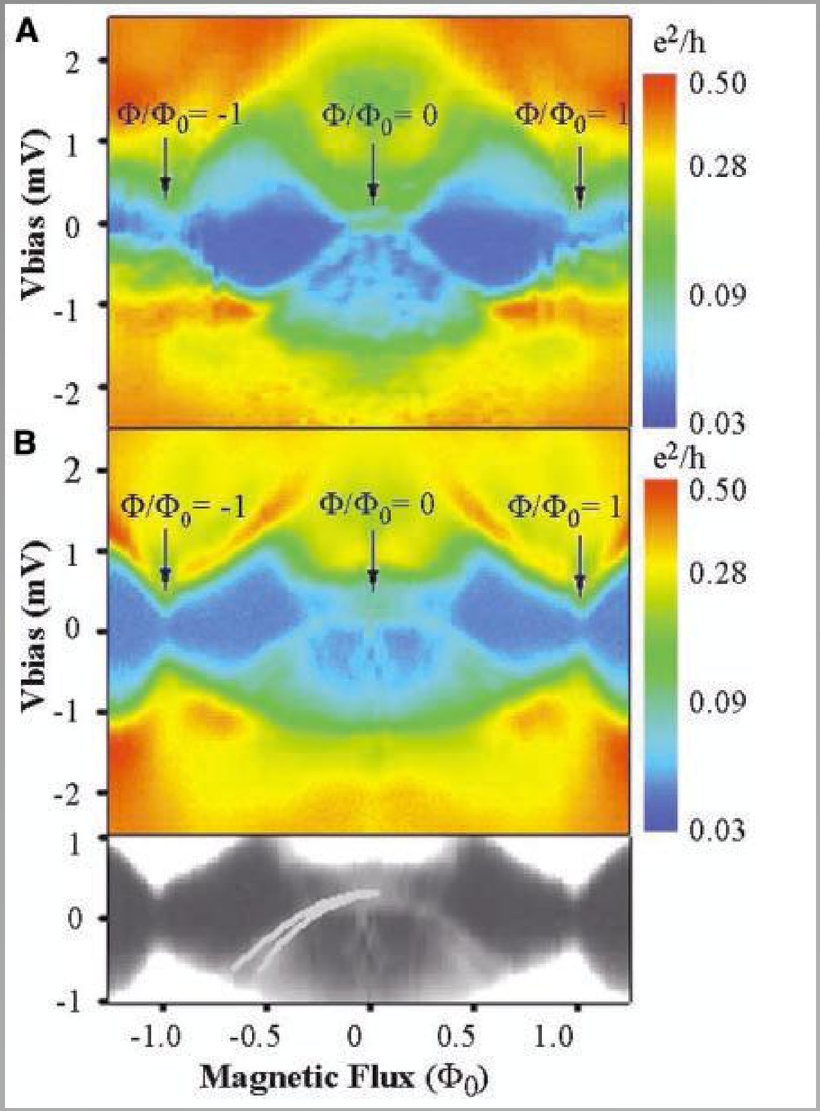


Coskun et al., Science 304 (2004) 1132

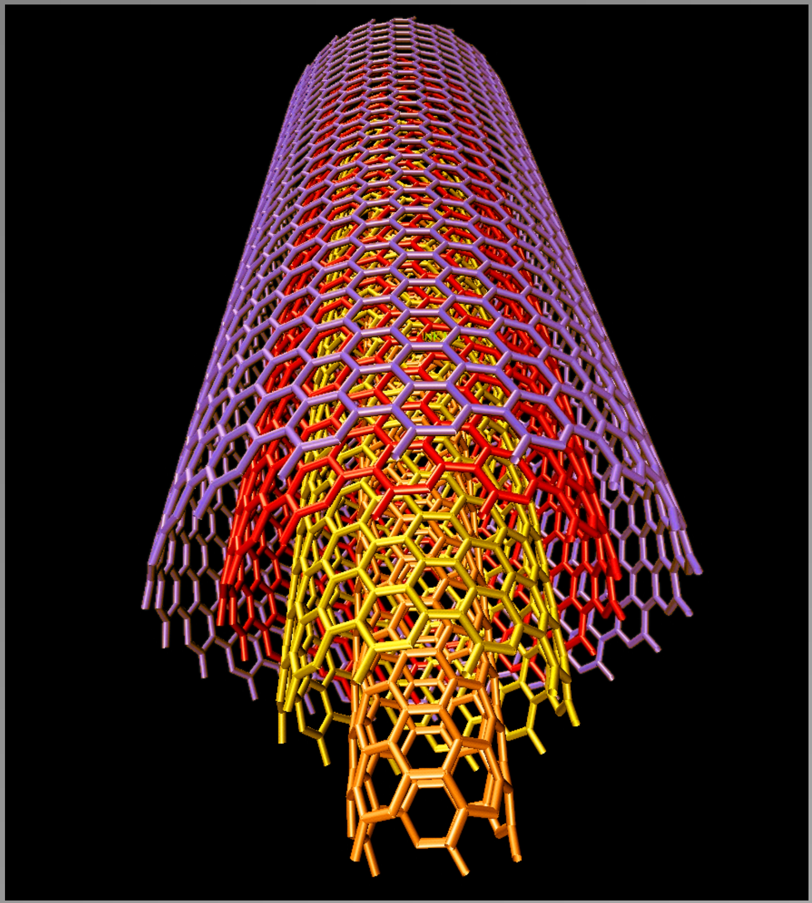
Aharonova-Bohm effect in multiwall nanotubes

- Periodic variation of conductance

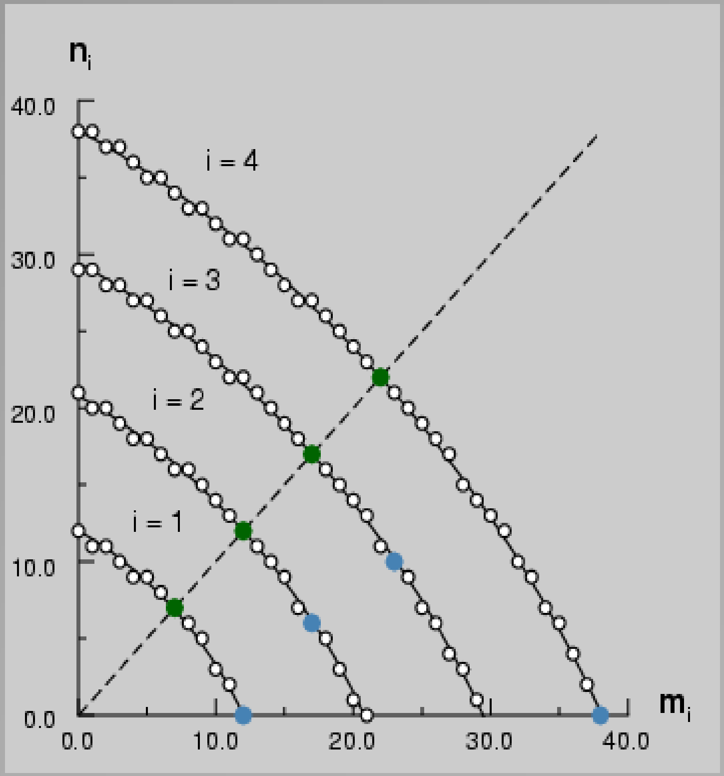
- Imperfect periodicity
  ⟶ a result of the magnetic response of inner nanotube shells?



Multiwall nanotubes, shell chiralities

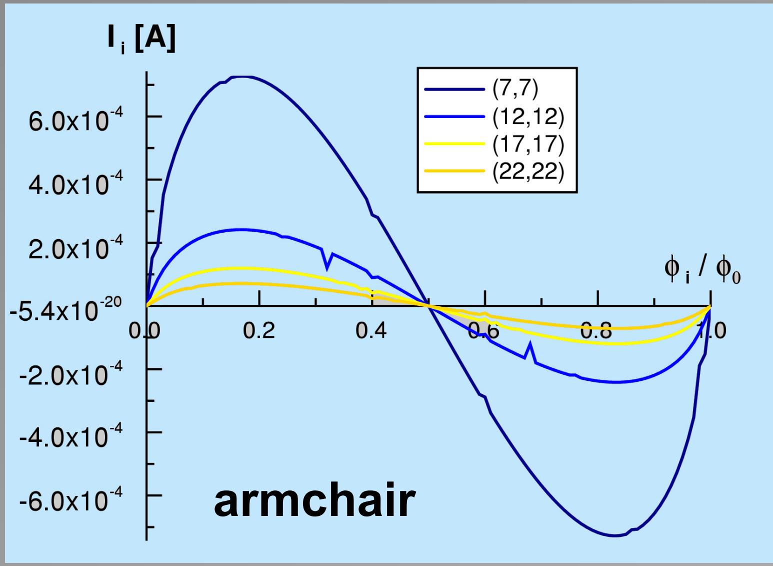


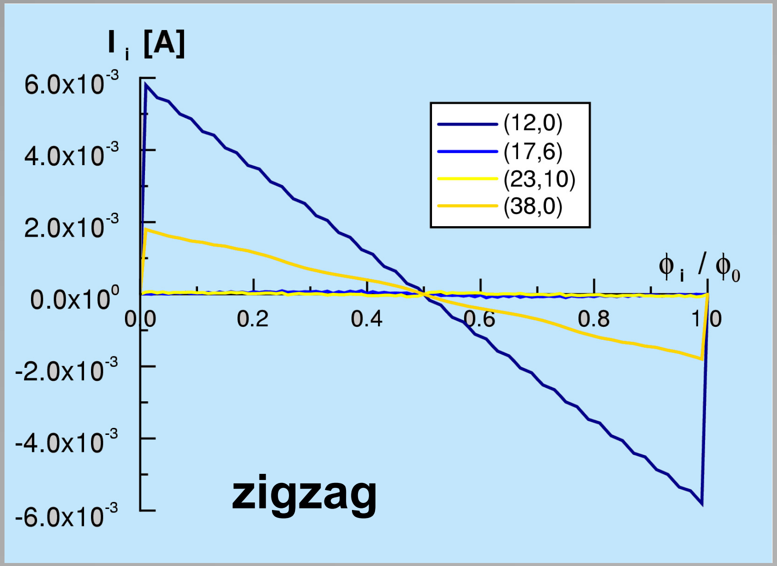
Possible shell chiralities may be found from the restriction on the intershell distance – it should be the same as in the turbostratic graphite, 3.4Å.



Optimal nanotube shell chiralities

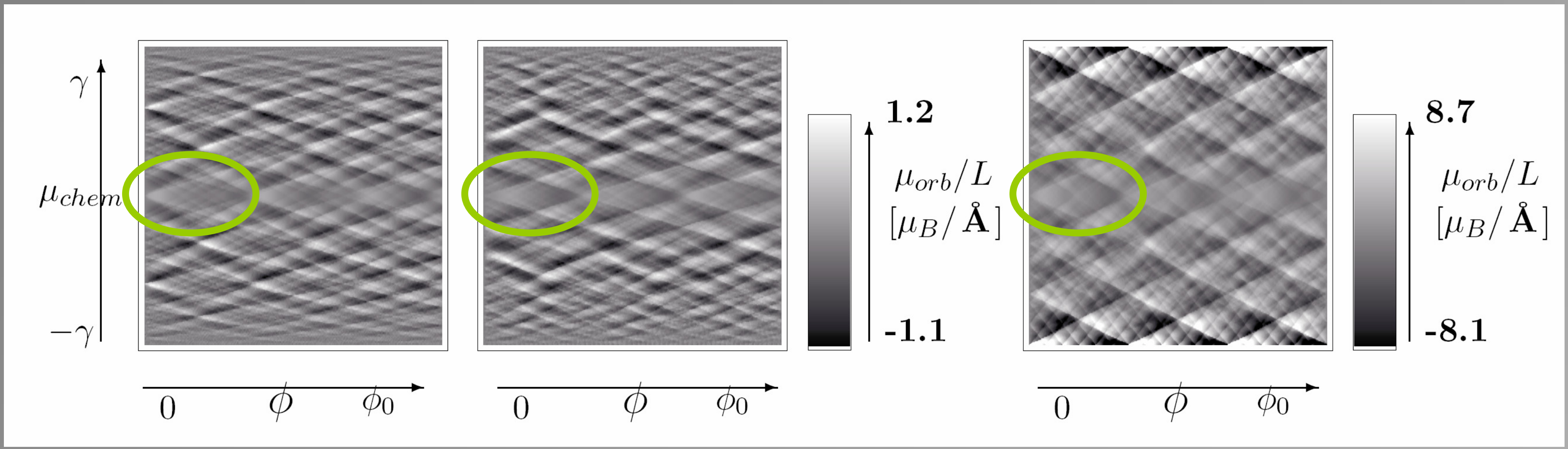
inner shell	configuration type	outer zigzag or armchair parameters	inter-shell distance
zigzag (m_1,0)	zigzag-zigzag	$(m_1+8,\ 0)$	3.13 Å
		$(m_1+9,\ 0)$	3.52 Å
	zigzag-chiral-zigzag	$(m_1+17,\ 0)$	3.32 Å
		$(m_1+18,\ 0)$	3.62 Å
	zigzag-chiral-chiral-zigzag	$(m_1+26,\ 0)$	3.39 Å
		$(m_1+27,\ 0)$	3.73 Å
armchair (m_1, m_1)	armchair, armchair	$(m_1+5,\ m_1+5)$	3.39 Å





Multiwall nanotubes – magnetic moment

armchair **chiral** **zigzag**



Outer radius: 15 Å, three inner shells

T = 0, μ = const

→ Complex periodicity

→ In a nanotube with outer zigzag shell, its contribution clearly dominates in the full magnetic moment.

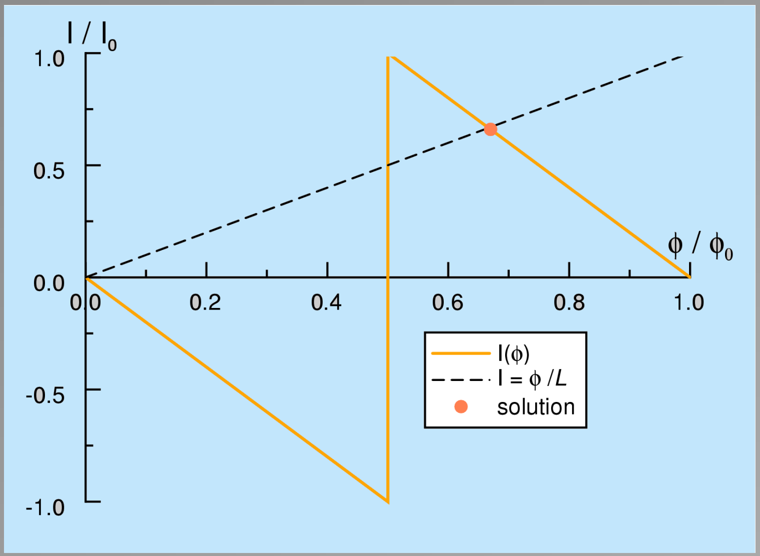
Trapped and spontaneous flux

M. Stebelski, M.S., E.Z., Z.Phys B 103 (1997) 79

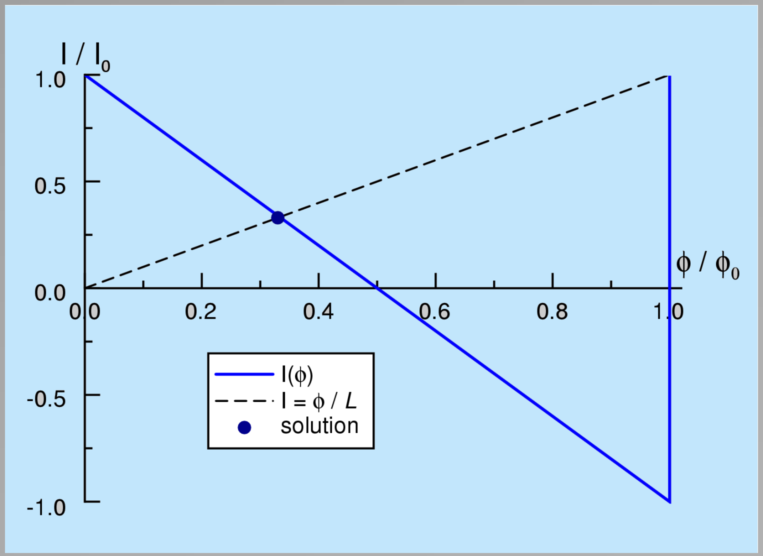
Persistent currents in the system induce a magnetic field which superposes with the external one.

$$\phi_t = \phi_e + \mathcal{L} I_t(\phi_t),$$

Together with the equation for the persistent current as the sum over momentum states, they form a pair of self-consistent equations which may have stable solutions.

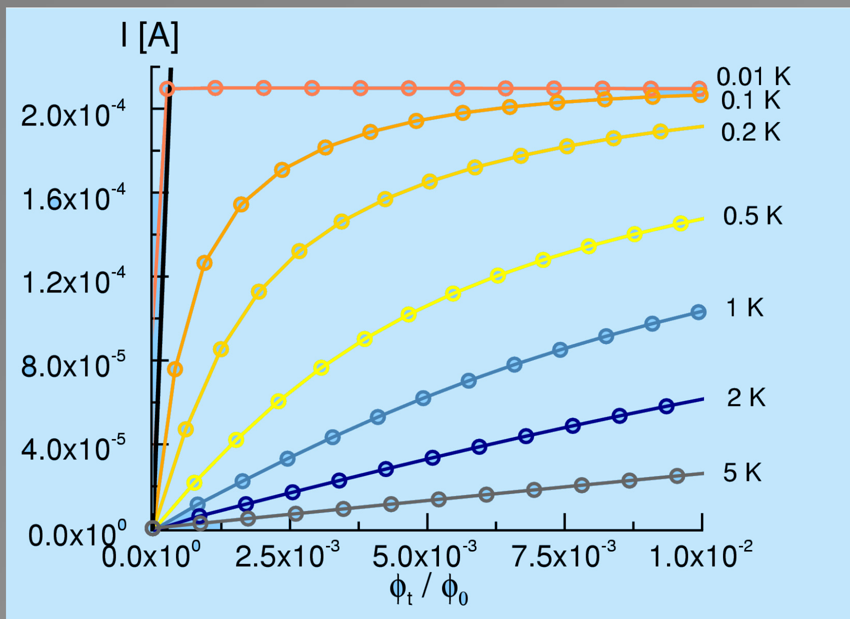


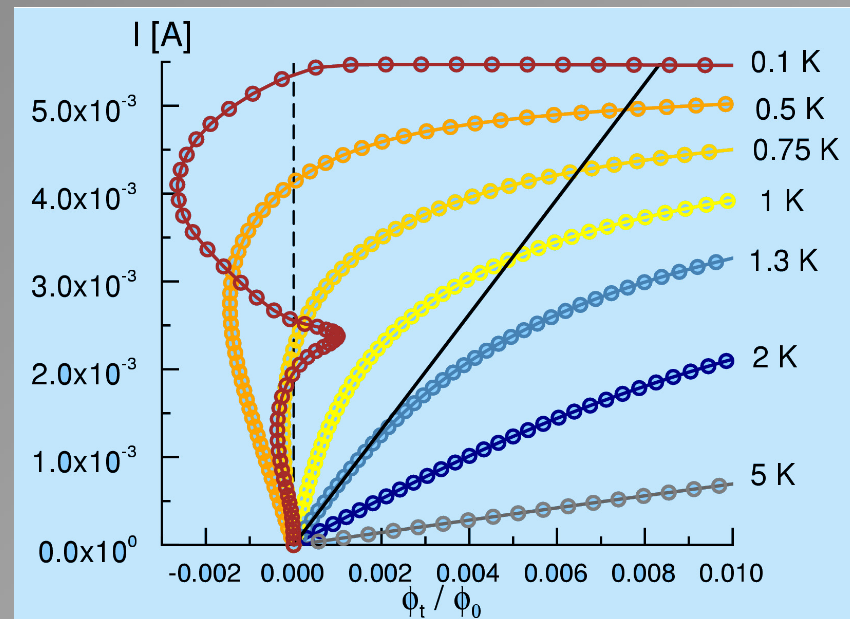
Trapped flux



Spontaneous flux

Spontaneous currents in multiwall nanotubes





Armchair, $\mu = 0$

R = 22nm
L = 1000 nm

54 active shells

Zigzag and chiral, $\mu = -\gamma$

R = 22nm
L = 1000 nm

18 active shells

Conclusions

Unusual disperion relation of graphene gives rise to several effects appearing in the presence of the magnetic field:

- Opening and closing of the energy gap in the nanotube in magnetic field $\longrightarrow$ a change of the nanotube's conduction type
- Independence of the magnetic moment of the nanotube radius, linear dependence in tubes doped to $-\gamma$
- Only two types of $\mu(\phi)$ dependence at small doping: metallic and semiconducting

Conclusions, continued

- At carefully chosen doping, strong enhancement of the nanotube's magnetic response
- In low temperatures $\longrightarrow$ spontaneous currents?
- Electron-hole symmetry at small μ, independent of temperature
- Possibility of determination of the π orbitals overlap through a measurement of the asymmetry at larger μ

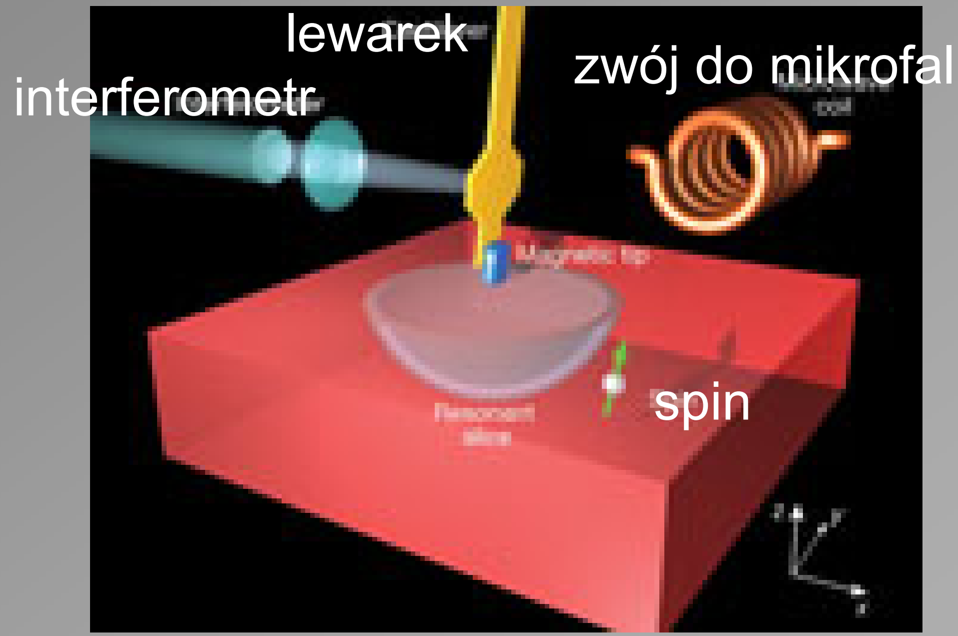
Phys. Lett. A 299 (2002)

Phys. Rev. B 70 (2004)

To appear in Phys. Rev. B 72 (2005)

Pytanie do ekspertów

Czy to się może udać?



„Single spin detection by magnetic resonance force microscopy", D. Rugar et al., Nature 430 (2004) 329