Spin orbit coupling in graphene & nanotubes

Reinhold Egger
Institut für Theoretische Physik
Universität Düsseldorf
Alessandro De Martino
Andreas Schulz
Karen Hallberg, Carlos Balseiro

HEINRICH HEINE
UNIVERSITÄT
DÜSSELDORF

Overview

- Introduction
- Theory of spin orbit coupling in graphene & carbon nanotubes
- Experimental evidence for spin orbit coupling in carbon nanotubes
- Consequences for transport in CNTs

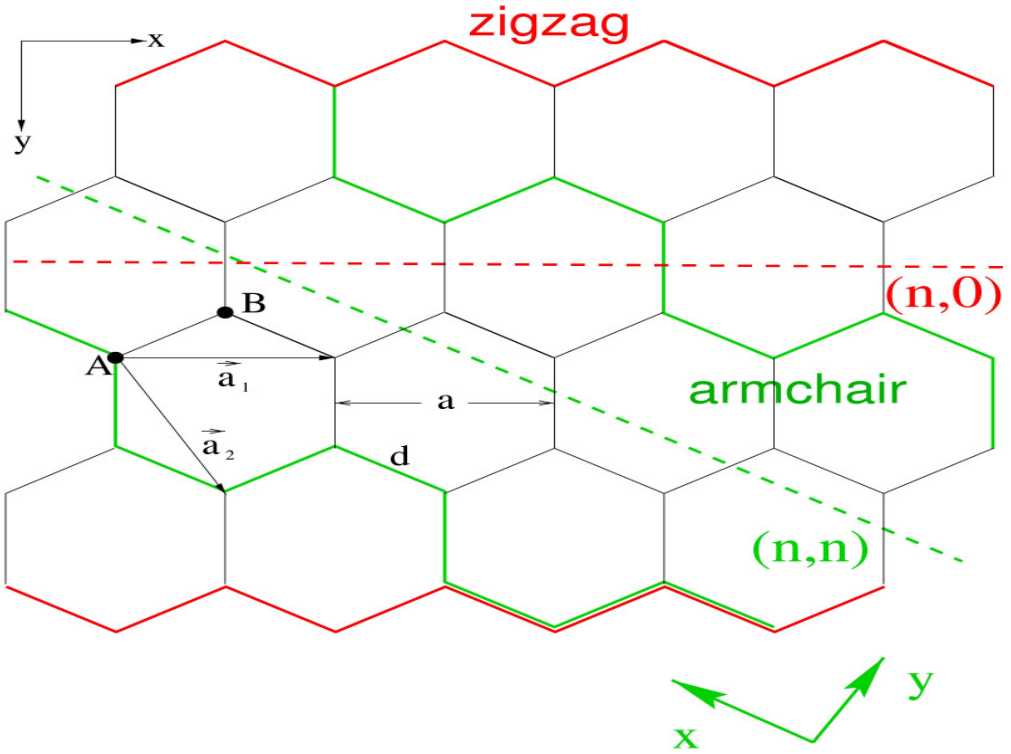
Graphene and carbon nanotubes

Basis contains two atoms (sublattices A and B)

$$a = \sqrt{3}d, d = 0.14nm$$

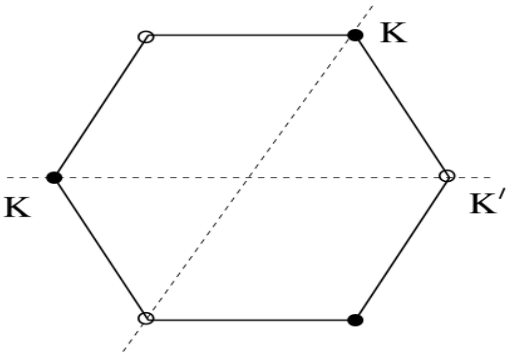
(n,m) indices: wrapping of sheet onto cylinder

Chiral angle θ: defined with respect to zigzag (n,0) tube



Band structure: Graphene

- Exactly two independent corner points K, K´ in first Brillouin zone.
- Band structure: valence and conduction bands touch at corner points *(E=0)*, these are the Fermi points in graphene
- Lowest-order k.p scheme: Dirac light cone dispersion
- Deviations: trigonal warping, spin orbit interactions, …



$$E(\vec{q}) = \pm v_F |\vec{q}|$$

$$\vec{q} = \vec{k} - \vec{K}$$

$$v_F \approx 10^6 \, m/\sec$$

Low energy theory

For energy scales close to K points, in leading order: massless 8-component Dirac spinor field $\tilde{\Psi}_{\alpha\sigma\tau}(x, y)$

$$H_0 = -i\hbar v_F \sum_{\alpha\sigma} \int d\vec{r}\ \tilde{\Psi}^{+}_{\alpha\sigma} \left[\tau_x \partial_x + \alpha\tau_y \partial_y\right] \tilde{\Psi}_{\alpha\sigma}$$

- Valley (KK´) index $\alpha = \pm$
- Sublattice index $\tau = \pm$ (with Pauli matrices in sublattice space)
- Spin $\sigma = \pm$

Spin orbit interaction (SOI)

- Electrons moving in electrostatic potential $\Phi(\vec{r})$ (due to ions or gate fields) experience effective magnetic field $\vec{B}_{eff} \propto \vec{v} \times \nabla\Phi$ in their rest system
- Second quantized formulation

$$H_{SOI} = \frac{g\mu_B}{4m} \int d\vec{r}\ \Psi^{+}\left[(\nabla\Phi \times \vec{p}) \cdot \vec{\sigma}\right]\Psi$$

- Expand field operator on honeycomb lattice

$$\Psi_{\sigma}(\vec{r}) = \sum_{j} \chi_{2p_z}\left(\vec{r} - \vec{r}_j\right) c_{j,\sigma}$$

Tight-binding form of SOI

De Martino, Egger, Hallberg & Balseiro, PRL 2002; JPCM 2004

$$H_{SOI} = i\sum_{j\neq k} c_j^{+}\left(\vec{u}_{jk}\cdot\vec{\sigma}\right) c_k + h.c.$$

with spin-orbit vectors

$$\vec{u}_{jk} = -\vec{u}_{kj} = \frac{g\mu_B}{4m}\int d\vec{r}\ \Phi(\vec{r})\left(\nabla\chi_{2p_z}\left(\vec{r}-\vec{r}_j\right)\times\nabla\chi_{2p_z}\left(\vec{r}-\vec{r}_k\right)\right)$$

Nearest-neighbor terms vanish by symmetry (integrand is odd under $z\leftrightarrow -z$) in ideal graphene:

intrinsic SOI comes from next-nearest neighbor terms & is therefore very small $(\Delta_{\text{int}} \approx 10\,mK)$

Curvature-induced SOI

- Nearest-neighbor terms are nonzero when external („Rashba“) electric fields or curvature-induced overlap changes break symmetry
- Curvature-induced SOI
  - Dominant SOI in absence of external field
  - Naturally present in carbon nanotubes
  - „Ripples“ may also generate this SOI in graphene
- Field-induced SOI
  - Graphene: analogue to Rashba SOI in semicond. 2DEG
  - Nanotubes: Rashba field gives small effect since it is averaged over circumference *De Martino & Egger, JPCM 2005*
  - Multiwall nanotubes: radial electric fields give interesting effects! *De Martino, Egger, Hallberg & Balseiro, PRL 2002*

Low energy SOI Hamiltonian: graphene

Ando, J.Phys.Soc.Jpn. 2002,
Huertas-Hernando, Guinea & Brataas, PRB 2006

- Connect $\Phi(\vec{r})$ to atomic SOI at carbon atom #*i*, $H_{SOI,i} = \lambda \vec{L}_i \cdot \vec{S}_i$
- Requires explicit inclusion of sp^2 orbitals into tight-binding model, which are perturbatively projected out to give SOI for π electrons
- Main benefit: numerical predictions for SOI couplings
- Structure of low-energy SOI theory: identical to results obtained from lattice representation

Final result

De Martino & Egger, JPCM 2005
Huertas-Hernando et al., PRB 2006

SOI interaction in graphene

$$H_{SOI} = (\Delta_{curv} + \Delta_E) \sum_{\alpha} \int d\vec{r}\ \tilde{\Psi}^{+}_{\alpha} (\tau_x \sigma_y + \alpha \tau_y \sigma_x) \tilde{\Psi}_{\alpha}$$

- tiny intrinsic contribution is omitted
- Curvature effects (ripples) and „Rashba“ electric field (perpendicular to graphene sheet) give same type of SOI term
- Carbon nanotubes: curvature due to wrapping to cylinder should give bigger SOI than in graphene

Low-energy theory for nanotube

- Introduce 1D spinors: $0 \le y < 2\pi R$

$$\tilde{\Psi}_{\alpha\sigma\tau}(x,y) = \sum_{n_0} \frac{e^{ik_{\perp n_0} y}}{\sqrt{2\pi R}} \psi_{n_0\alpha\sigma\tau}(x)$$

- Unitary transformation from sublattice description to right/left movers

$$\tau_x \to \tau_z, \quad \tau_y \to \tau_x$$

- „Free theory“: Multimode quantum wire

$$H_0 = \sum_{n_0\alpha\sigma} \hbar v_F \int dx \; \psi^+_{n_0\alpha\sigma} \left(-i\tau_z \partial_x + \alpha k_{\perp n_0} \tau_x \right) \psi_{n_0\alpha\sigma}$$

Bandstructure of carbon nanotube

2D Dirac spinor obeys twisted boundary condition around circumference: $\vec{T} = n\vec{a}_1 + m\vec{a}_2$

$$\tilde{\Psi}_\alpha\left(\vec{r}+\vec{T}\right) = e^{i\alpha\frac{2\pi\nu}{3}}\tilde{\Psi}_\alpha\left(\vec{r}\right)$$

$$\vec{T}\cdot\vec{K} = 2\pi\nu/3$$

$$\nu = \mathrm{mod}(2n+m,3) = 0,\pm 1$$

↷ 1D bands (integer n_0) with transverse momentum $k_\perp R = n_0 - \alpha\nu/3$ and longitudinal momentum *k:*

$$E_{n_0\alpha\sigma}(k) = \pm\hbar v_F\sqrt{k^2 + k_\perp^2}$$

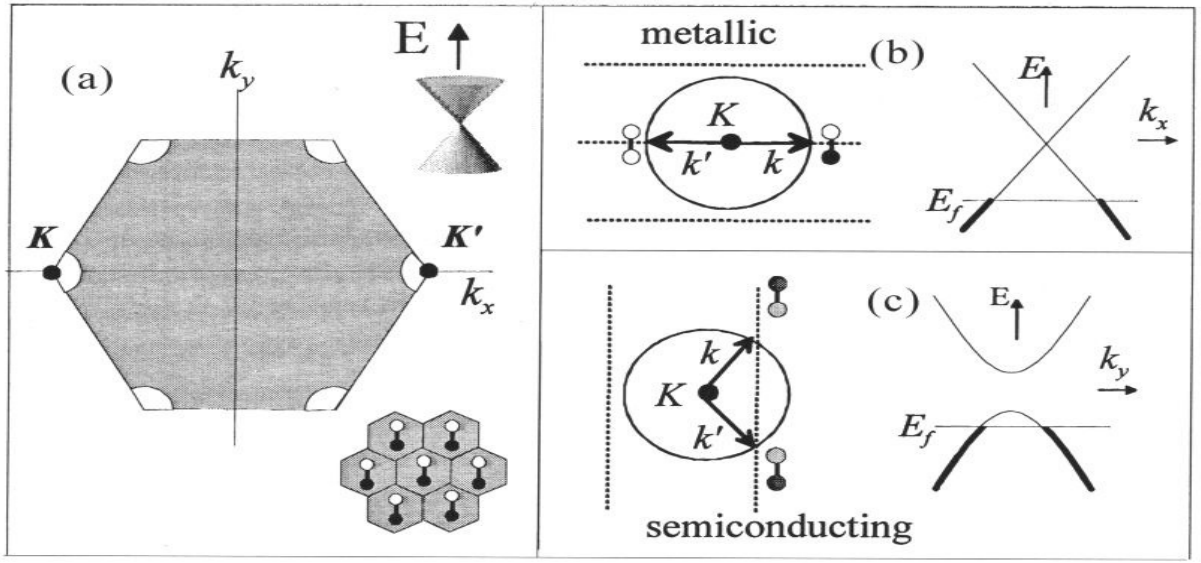
metallic only for $n_0 = \nu = 0$

Periodic boundary conditions

Transverse momentum must be quantized

Nanotube metallic only if K point has allowed transverse momentum

gives necessary condition: *2n+m = 3 x* integer



Curvature SOI in SWNT

Ando, JPSJ 2000
De Martino & Egger, PRL 2002

- Leading contribution (spin quantization axis along *x*)

$$H_{SOI} = \Delta_{curv} \sum_{\alpha\sigma} \alpha\sigma \int dx \; \psi^{+}_{n_0\alpha\sigma} \tau_x \psi_{n_0\alpha\sigma}$$

  - No spin flip
  - Can be included as a spin-dependent topological flux $\sigma\phi_{SO}$ into transverse momentum
- Subleading contribution (from second term)
  - Requires mixing of subbands $n_0 \Leftrightarrow n_0 \pm 1$
  - Then spin flips occur (contribution to spin relaxation rate)
  - Similar as in semiconductor quantum wires with Rashba spin-orbit coupling *Governale & Zülicke, SSC 2004*

Including curvature effects & parallel magnetic field (AB flux), transverse momentum is quantized as

$$k_\perp R = n_0 - \frac{\alpha\nu}{3} + \frac{\phi_{AB} + \sigma\phi_{SO}}{\phi_0} + \alpha\frac{\kappa a}{R}\cos(3\theta)$$

AB and SO flux. Topological fluxes (in units of flux quantum)

Curvature term, depends on chiral angle, with

$$\kappa \approx 0.1$$

$$\frac{\phi_{SO}}{\phi_0} = \frac{\Delta_{curv} R}{\hbar v_F} \approx 10^{-3}$$

Ando, JPSJ 2002

SOI in CNTs small – is it observable?

Bandstructure of CNT

With trigonal warping corrections (up to Zeeman shift):

complete low-energy bandstructure of CNT

$$E_{n_0\alpha\sigma}(k) = \pm\hbar v_F \sqrt{k^2 + k_\perp^2 - \frac{\alpha a}{2\sqrt{3}}\left[\cos(3\theta)\left(k_\perp^3 - 3k_\perp k^2\right) + \sin(3\theta)\left(k^3 - 3kk_\perp^2\right)\right]}$$

- ✓ Kramers time-reversal symmetry for *B=0:*

$$E_{-n_0,-\alpha,-\sigma}(-k) = E_{n_0\alpha\sigma}(k)$$

- ✓ In achiral CNT also: $E_{n_0\alpha\sigma}(-k) = E_{n_0\alpha\sigma}(k)$

$$\left(\theta = 0, \pi/6\right)$$

Spin splitting for zero magnetic field

- In nanotube dot, level splitting due to SOI occurs even in absence of magnetic field
- Estimate (k=0):
  - States with (anti-)parallel pseudospin and spin (i.e. for same $\alpha\sigma=\pm 1$) remain (Kramers) degenerate
  - SOI splitting between parallel and antiparallel states is

$$\Delta_{SO} = \frac{2\hbar v_F}{R}\frac{\phi_{SO}}{\phi_0} \approx \frac{0.8\,meV}{R\,[nm]}$$

  - Experimentally observed via Coulomb blockade spectroscopy for clean one-electron nanotube dot

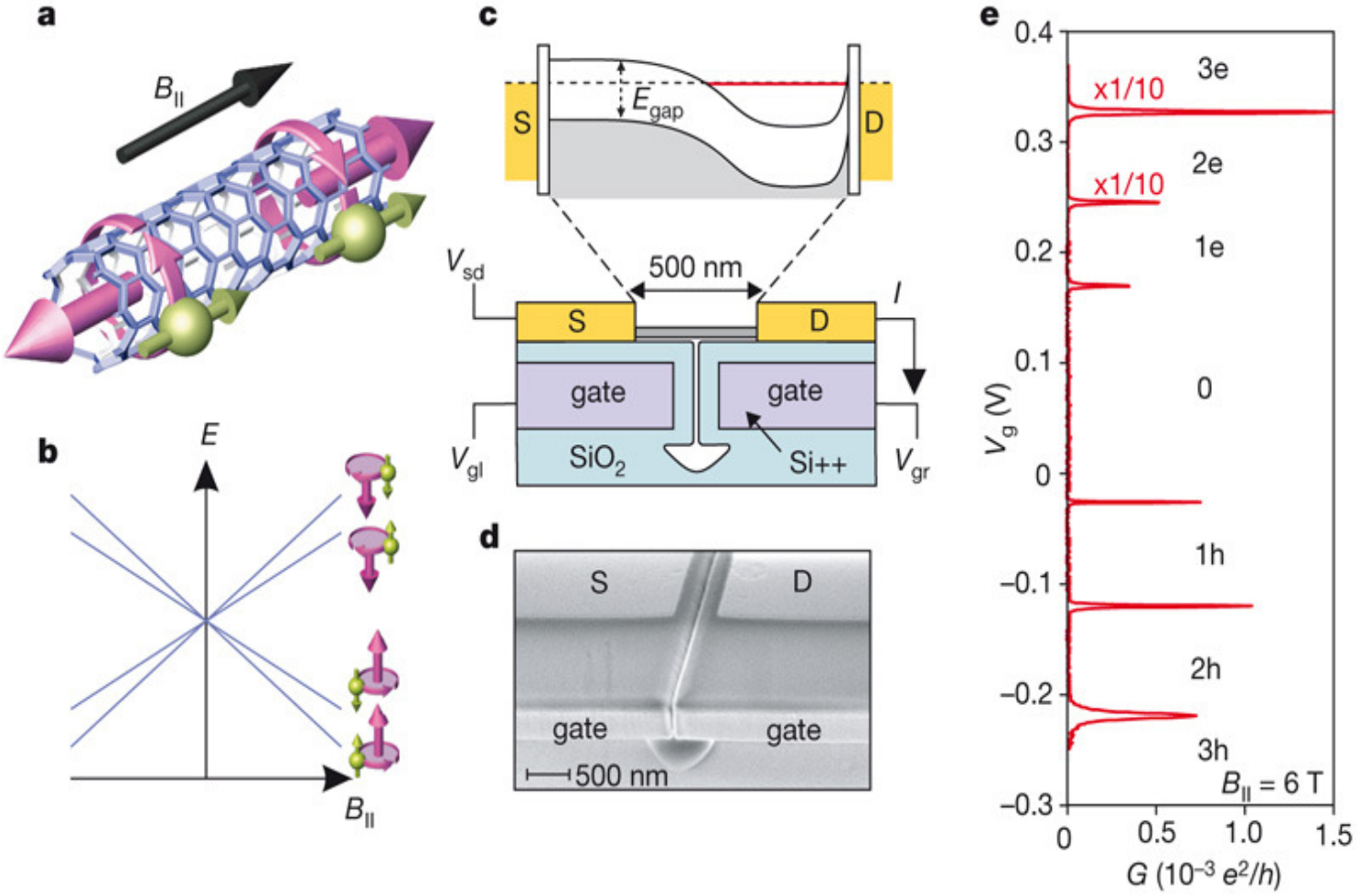
Kuemmeth, Ilani, Ralph & McEuen, Nature 2008

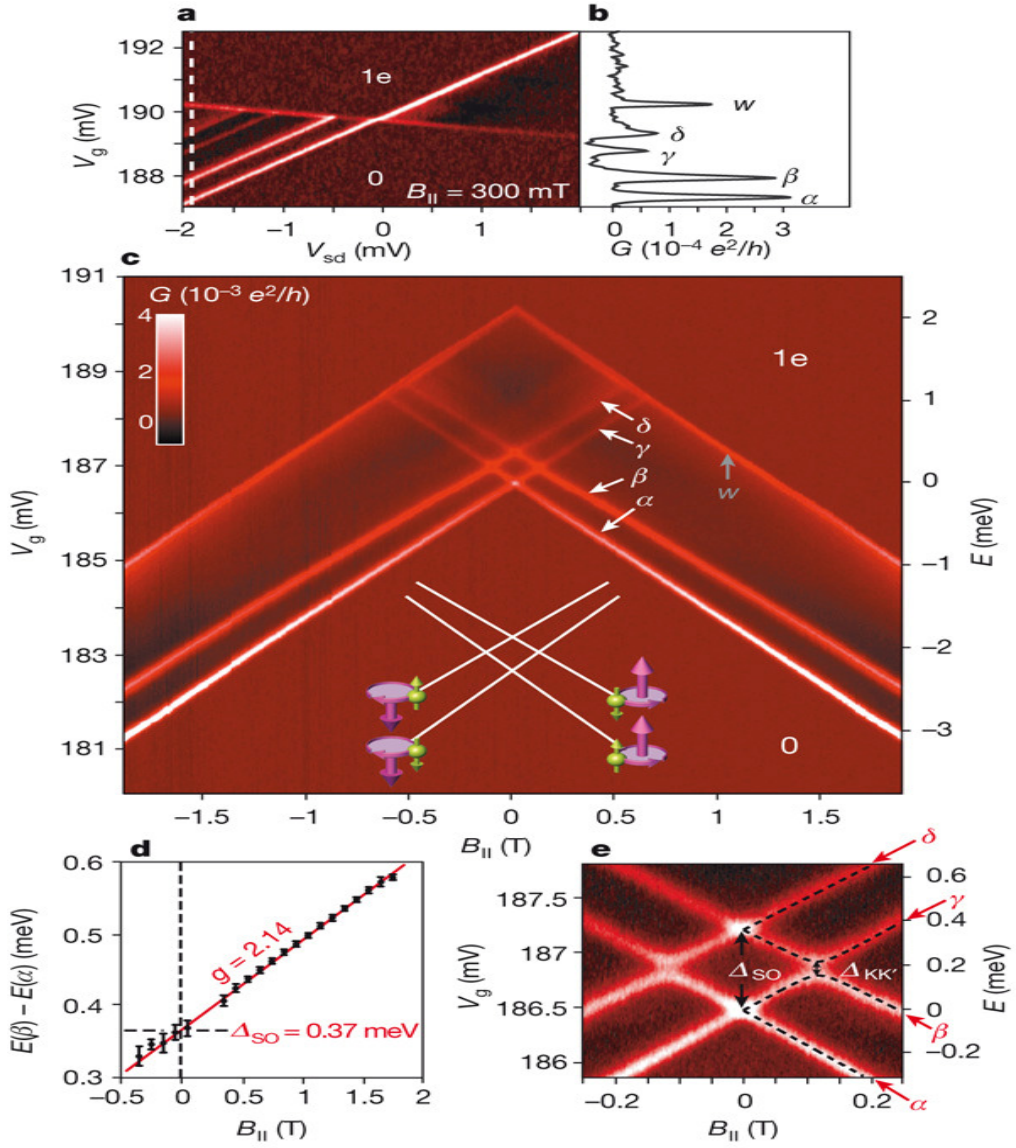
Experiment

$R \approx 2.5nm$

$\nu = 0$

Kuemmeth et al., Nature 2008





Direct measurement of single-particle levels via finite-bias cuts in Coulomb Blockade spectroscopy

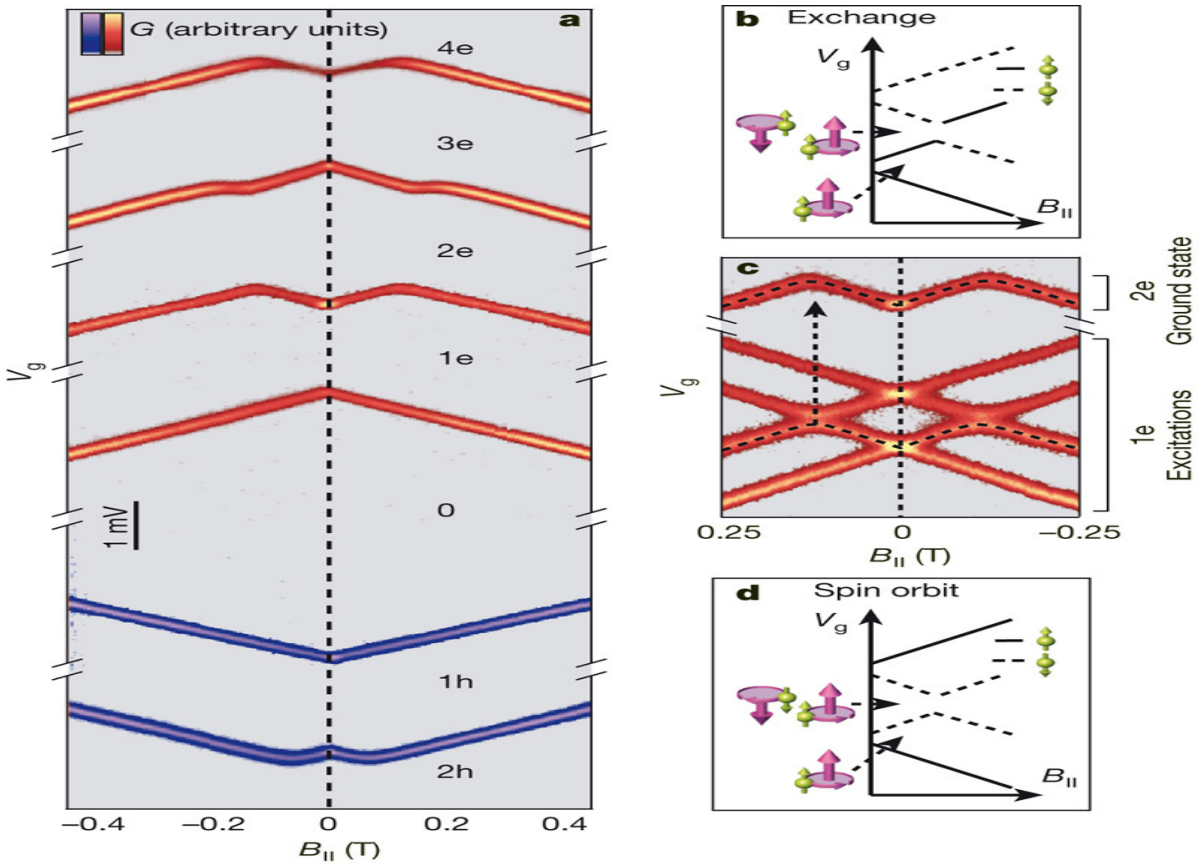
SO splitting in zero field observed:

$$\Delta_{SO} \approx 0.37 meV$$

Ultraclean CNT, almost no KK‘ mixing

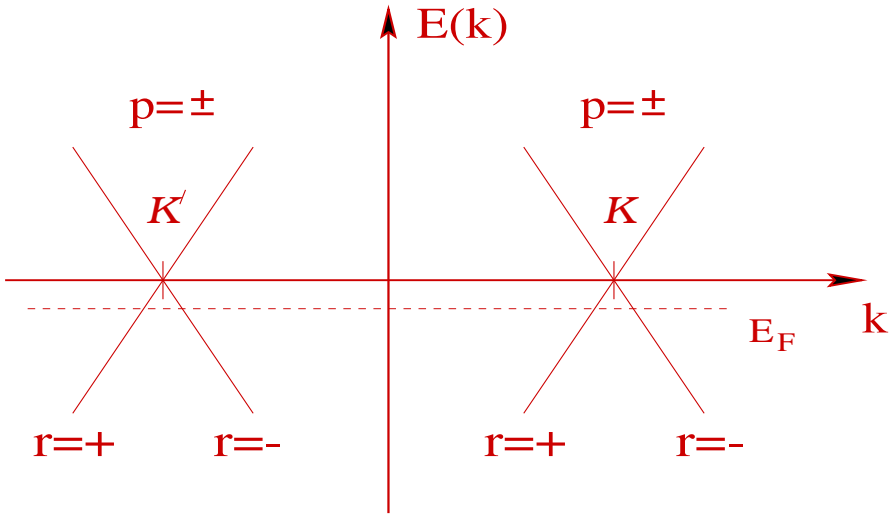
Also affects spin configuration of many-electron dots…

Kuemmeth et al., Nature 2008



Interactions in metallic SWNTs

Standard picture (ignoring SOI corrections)



- Transverse momentum quantization: keep only $k_\perp = 0$
- Ideal 1D quantum wire: 2 spin-degenerate bands
- Low-energy theory: restrict to these 2 bands, but include (long-ranged) Coulomb interactions

Egger & Gogolin, PRL 1997, EPJB 1998
Kane, Balents & Fisher, PRL 1997

Bosonized form

Four bosonic fields, index $a = c+, c-, s+, s-$

Low-energy theory: Luttinger liquid

$$H = \sum_a \frac{v_a}{2} \int dx \left[g_a \Pi_a^2 + g_a^{-1} (\partial_x \varphi_a)^2 \right]$$

$$g_{a \neq c+} \cong 1 \qquad g \equiv g_{c+} \approx 0.2$$

$$v_{c+} = v_F / g, \; v_{a \neq c+} = v_F$$

exactly solvable Gaussian model, leads to spin-charge separation. Experimental evidence from tunneling density of states etc. available!

SOI effects on Luttinger liquid

- Broken spin SU(2) symmetry: Fermi velocities depend on spin, K point and direction ($r=R/L=\pm$)
- For $B=0$:

$$\frac{v_F^{(\alpha\sigma r)}}{v_F} = 1 - \alpha\sigma\left(\gamma + r\sigma\eta\right)$$

$$\gamma = \frac{\kappa a \phi_{SO}}{k_F^2 R^3 \phi_0}\cos(3\theta) \qquad \eta = \frac{k_F a}{4\sqrt{3}}\sin(3\theta)$$

- For $\gamma\eta\neq 0$, this couples spin and charge sector: SOI implies breakdown of spin-charge separation
  - happens only for chiral tubes, $\sin(6\theta)\neq 0$
  - affects observables probing spin-charge separation: ESR, spin transport, momentum-resolved tunneling,…

Balents & Egger, PRB 2001; De Martino & Egger, EPL 2001

Luttinger liquid with broken spin-charge separation

Schulz, De Martino, Ingenhoven & Egger, arXiv:0902.4402

- Modification of Luttinger theory due to SOI in chiral tubes necessary: spin-charge mixing terms
- Remains Gaussian model, exactly solvable
- Power laws for tunneling density of states are changed & explicitly depend on SO coupling!

Conclusions

- Spin orbit couplings in nanotubes observable and significant (but expected to be small in graphene)
- Interesting consequences for effective low-energy theory of carbon nanotubes: modified Luttinger liquid with broken spin-charge separation