Spin orbit coupling in graphene & nanotubes

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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)

\( a = \sqrt{3}d, \quad d = 0.14\text{nm} \)

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

Chiral angle \( \theta \): 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
  \[ E(\vec{q}) = \pm v_F |\vec{q}| \]
  \[ \vec{q} = \vec{k} - \vec{K} \]
  \[ v_F \approx 10^6 \text{ m/sec} \]
- Deviations: trigonal warping, spin orbit interactions, …
Low energy theory

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

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

- 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

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

- Expand field operator on honeycomb lattice

$$\Psi_{\sigma}(\vec{r}) = \sum_j \chi_{2p_z} (\vec{r} - \vec{r}_j) c_{j,\sigma}$$
Tight-binding form of SOI

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

\[ H_{\text{SOI}} = i \sum_{j \neq k} c_j^+ (\tilde{u}_{jk} \cdot \sigma) c_k + \text{h.c.} \]

with spin-orbit vectors

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

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 \( (\Delta_{\text{int}} \approx 10mK) \)
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

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 $\pi$ electrons
- Main benefit: numerical predictions for SOI couplings
- Structure of low-energy SOI theory: identical to results obtained from lattice representation
Final result

SOI interaction in graphene

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

- 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

De Martino & Egger, JPCM 2005
Huertas-Hernando et al., PRB 2006
Low-energy theory for nanotube

- Introduce 1D spinors: \( 0 \leq y < 2\pi R \)
  \[
  \tilde{\Psi}_{\alpha \sigma \tau}(x, y) = \sum_{n_0} \frac{e^{ik_{\perp n_0} y}}{\sqrt{2\pi R}} \psi_{n_0 \alpha \sigma \tau}(x)
  \]

- Unitary transformation from sublattice description to right/left movers
  \[\tau_x \rightarrow \tau_z, \quad \tau_y \rightarrow \tau_x\]

- „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:  \[ \vec{T} = n\vec{a}_1 + m\vec{a}_2 \]
\[ \tilde{\Psi}_\alpha(\vec{r} + \vec{T}) = e^{i\frac{2\pi\nu}{3}} \tilde{\Psi}_\alpha(\vec{r}) \]
\[ \vec{T} \cdot \vec{K} = 2\pi\nu / 3 \]
\[ \nu = \text{mod}(2n + m,3) = 0,\pm1 \]

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: $2n+m = 3 \times \text{integer}$
Curvature SOI in SWNT

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 \( \kappa \approx 0.1 \)

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

SOI in CNTs small – is it observable?

Ando, JPSJ 2002
Bandstructure of CNT

With trigonal warping corrections (up to Zeeman shift):

complete low-energy bandstructure of CNT

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

✔ Kramers time-reversal symmetry for \( B=0 \):

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

✔ In achiral CNT also:

\[ E_{n_0\alpha\sigma}(-k) = E_{n_0\alpha\sigma}(k) \quad (\theta = 0, \pi/6) \]
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 $\alpha\sigma=\pm1$) 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

$R \approx 2.5 \text{nm}$

$\nu = 0$

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:

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

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

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

\[
g_{a \neq c^+} \equiv 1 \quad g \equiv g_{c^+} \approx 0.2
\]

\[
\nu_{c^+} = \frac{\nu_F}{g}, \quad \nu_{a \neq c^+} = \nu_F
\]

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 \(B=0\):
  \[
  \gamma = \frac{\kappa a \phi_{SO}}{k_F^2 R^3 \phi_0} \cos(3\theta) \\
  \eta = \frac{k_F a}{4\sqrt{3}} \sin(3\theta)
  \]

- 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

- 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