Spin orbit interaction in graphene monolayers & carbon nanotubes

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Overview

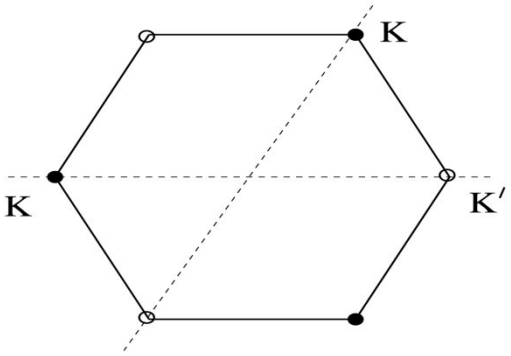
- Introduction: theory of spin orbit interaction (SOI) in graphene monolayer
- Landau levels and edge states in graphene with enhanced SOI

  A. De Martino, A. Hütten, RE, PRB 84, 155420 (2011)
- Consequences of SOI for Luttinger liquid description of metallic interacting nanotubes

  A. Schulz, A. De Martino, RE, PRB 82, 033407 (2010)

Band structure: Graphene

- Two independent K points in first Brillouin zone: „valley“ d.o.f.
- Band gap vanishes at K points (Dirac points, E=0)
- Lowest-order **k.p** scheme: „relativistic“ Dirac light cone dispersion close to Dirac point
- Additional terms arise (e.g.) from
  - Spin orbit coupling
  - High energies: trigonal warping (neglected here)



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

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

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

Massless Dirac fermions

Dirac spinor field $\Psi_{\alpha\sigma\tau}(x,y)$

$$H_0 = \sum_{\alpha\sigma} \int d\vec{r}\ \Psi^{+}_{\alpha\sigma}\, h_0 \Psi_{\alpha\sigma}$$

$$h_0 = -i\hbar v_F(\alpha\tau_x\partial_x + \tau_y\partial_y)$$

- Valley α=± , spin σ=± , sublattice $\tau = \pm$
  - Here: Pauli matrices in sublattice space
- Now add SOI:

$$h_0 \rightarrow h_0 + h_{SOI}$$

Spin orbit interaction (SOI)

- Electrons moving in electrostatic potential $\Phi(\vec{r})$ feel effective magnetic field $\vec{B}_{eff} \propto \vec{v} \times \nabla\Phi$ in their rest system (relativistic correction)
- Second quantized formulation

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

- 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↔ –z) in ideal graphene:

Intrinsic SOI comes from next-nearest neighbor terms & is very small $(\Delta \approx 10mK)$

„Rashba“ type SOI

- Nearest-neighbor terms finite when external („Rashba“) electric field (substrate, gate) or curvature-induced overlap breaks this symmetry
- Curvature-induced SOI
  - Naturally present in carbon nanotubes
  - „Ripples“ may also generate it in graphene
- Field-induced SOI
  - Cf. Rashba SOI in semicond. 2DEG
  - Nanotubes: Rashba field gives small effect since it is averaged over circumference *De Martino & Egger, JPCM 2005*
  - MWNTs: radial electric fields may 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 i.th atom:

$$H_{SOI,i} = \lambda_0 \vec{L}_i \cdot \vec{S}_i$$

- 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 can also be obtained from lattice representation

SOI interaction in graphene

$$h_{SOI} = \Delta\ \alpha\tau_z\sigma_z + \frac{\lambda}{2}\left(\alpha\tau_x\sigma_y - \tau_y\sigma_x\right)$$

spin Pauli matrices

- Δ: intrinsic SOI
- λ : „Rashba“ SOI (curvature, electric field)
- Enhancement of pristine (small) values:
  - *Ab initio* calculations: Indium or Thallium adatom deposition yields up to Δ≈100 K

    Weeks et al., arXiv:1105.3282
  - Graphene experiments on Ni surfaces report large values for λ

    Varykhalov et al., PRL 2008

Kane-Mele model: „quantum spin Hall“ (QSH) phase

Kane & Mele, PRL 2005

- Topological insulator for $\Delta > \lambda/2$: bulk band gap but gapless excitations at boundary
- Helical edge liquid : right- and left-moving states have opposite spin polarization
  - Spin-independent impurity backscattering strongly suppressed
- Observed in HgTe wells *König et al., J.Phys.Soc.Jpn. 2008*
- Possibility to study QSH phase in graphene!
  - Here: what happens in a perp. magnetic field?

Graphene band structure with SOI and magnetic field

Hütten, De Martino & Egger, PRB 2011

- Consider piecewise constant magnetic field B
  - Cyclotron orbits: magnetic length $l = \sqrt{\hbar c / 2eB}$
  - Energy scale $\hbar\omega_c = \hbar v_F / l \sim \sqrt{B}$

    B=1T: ≈ 36 meV (l ≈ 18 nm)
  - Also include spin Zeeman energy

    $$E_Z = g\mu_B B << \hbar\omega_c$$
- Exact spinor eigenstates available

  in terms of parabolic cylinder functions of order p

Homogeneous field: Landau levels

Normalizability: p=n=0,1,2,3,… ⟹ Landau levels solve the quartic equation

$$\left[(E+E_Z)^2-n(\hbar\omega_c)^2-\Delta^2\right]\left[(E-E_Z)^2-(n+1)(\hbar\omega_c)^2-\Delta^2\right]$$
$$=\lambda^2\left[(E-\Delta)^2-E_Z^2\right]$$

- Standard result for $\Delta=\lambda=E_Z=0$: $E_{\pm,n}=\pm\hbar\omega_c\sqrt{n}$
- Recover $\Delta=E_Z=0$ results *Rashba, PRB 2009*
- General case: no zero modes in presence of SOI
- Particle hole symmetry broken for $E_Z\neq 0\cup\lambda\Delta\neq 0$
- Exact solution for n=0 and spin down:

$$E_{n=0,\downarrow}=\Delta-E_Z$$

QSH phase without time reversal symmetry

- Quartic equation can be solved analytically, but expressions lenghty & not illuminating
- Study fate of QSH phase in the magnetic field for simpler limit λ=0 : QSH phase for B=0
  - Can QSH phase survive time reversal symmetry breaking (B>0)? *Yang et al., PRL 2011*
- Then spin σ conserved, quartic eqn yields

$$E_{\pm,n,\sigma} = \sigma E_Z \pm \sqrt{n(\hbar\omega_c)^2 + \Delta^2}$$

  - no zero mode: $E_{0,\sigma} = \sigma(E_Z - \Delta)$

Edge states (for $\lambda=0$)

- Semi-infinite geometry y<0 with armchair boundary condition at y=0
  - Wavenumber k_x conserved
  - For $k_x < 0$: distance from boundary set by $|k_x|$
- Order p of cylinder function now arbitrary real
  - determined by boundary condition (symmetric or antisymmetric valley combinations)

$$\left(\sqrt{p(\hbar\omega_c)^2+\Delta^2} \mp \sigma E_Z\right) D_{p-1}(2k_x l) + \hbar\omega_c D_p(2k_x l) = 0$$

  - Dispersion relation: $E_{\pm,\sigma}(k_x) = \sigma E_Z \pm \sqrt{p(k_x)\,(\hbar\omega_c)^2+\Delta^2}$

Edge states

- Standard chiral Hall edge states are recovered for Δ=0
- Generalized QSH phase with helical edge liquid near Dirac point for $\Delta > E_Z$

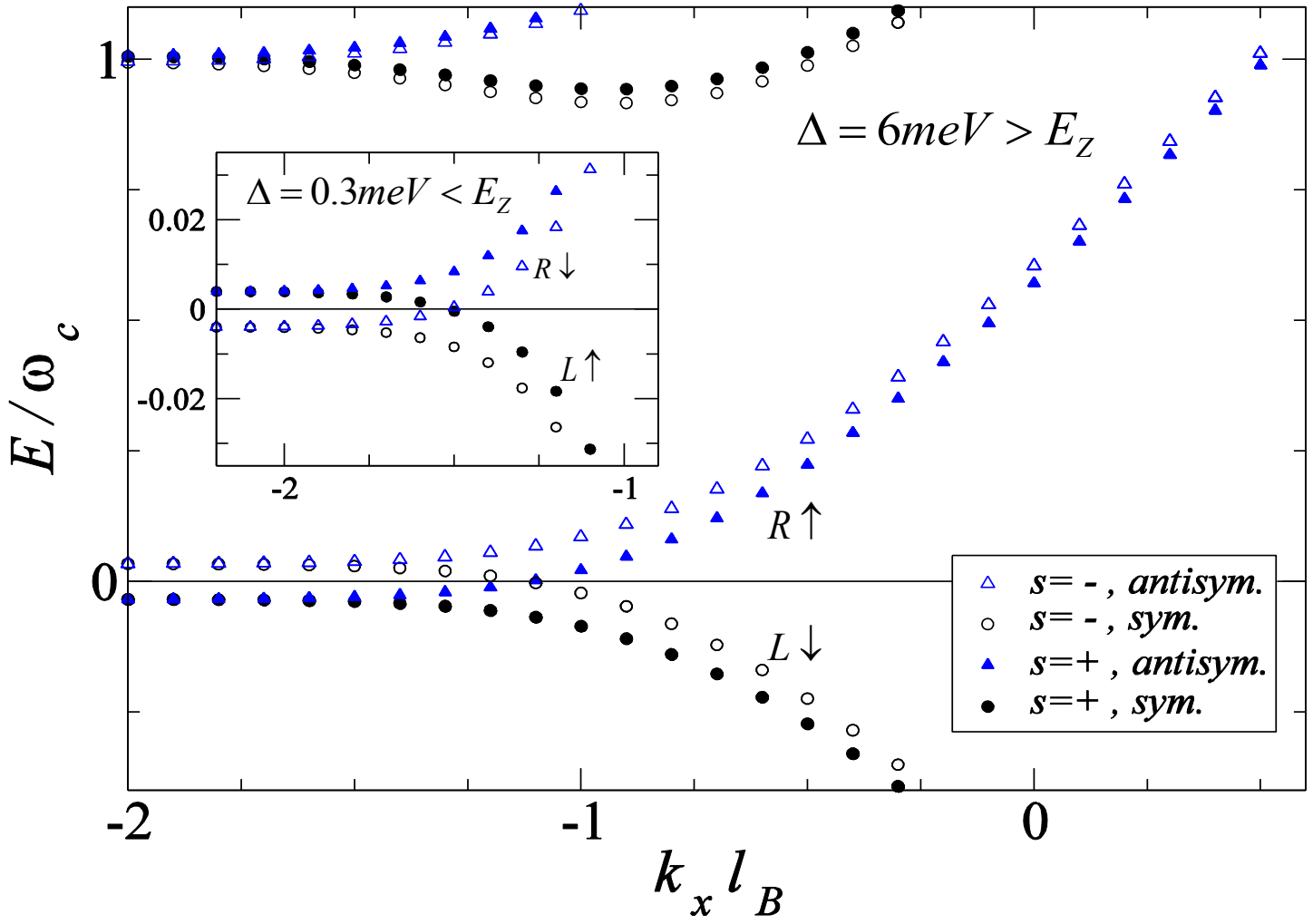
Kane & Mele, PRL 2005, Yang et al., PRL 2011

- Quantum phase transition at $\Delta = E_Z$
- Spin-filtered Hall edge state for $\Delta < E_Z$

Abanin, Lee & Levitov, PRL 2006

- Both phases similar but with opposite spin current!

Edge states: numerical solution



Conclusion Part I

- Full set of Landau states and energies for arbitrary SOI and Zeeman energy
  - Zero mode disappears (spin splitting)
  - Only valley degeneracy remains
  - Particle hole symmetry usually broken
- Generalized QSH phase (with broken time reversal symmetry) possible for large Δ
  - topological insulator with spin-filtered helical edge states realizable in graphene with Th or In adatoms

A. De Martino, A. Hütten & RE, PRB 84, 155420 (2011)

Bandstructure of carbon nanotube

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

$$\Psi_\alpha\left(\vec{r} + \vec{T}\right) = e^{i\alpha\frac{2\pi\nu}{3}}\Psi_\alpha\left(\vec{r}\right) \qquad \vec{T}\cdot\vec{K} = 2\pi\nu/3$$

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

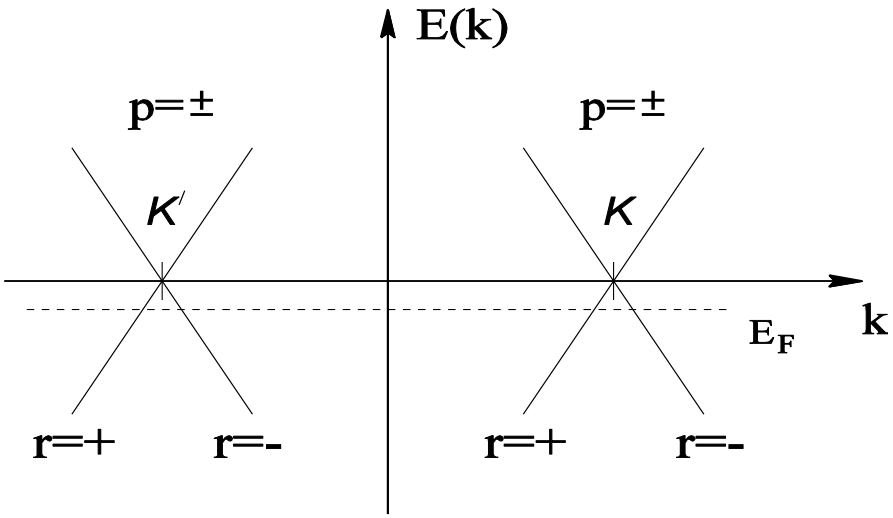
1D bands (integer n_0) with transverse momentum $k_\perp R = n_0 - \alpha\nu/3$ and longitudinal momentum k:

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

metallic: $n_0 = \nu = 0$

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

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

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

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

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

SOI in metallic SWNT

Ando, JPSJ 2000
Schulz et al., PRB 2010

- How to produce SWNT with enhanced SOI unclear
  - omit tiny intrinsic SOI (Δ)
  - estimate „Rashba“ SOI (λ) for clean tube
- Dominant curvature-induced SOI *Izumida et al., JPSJ 2009*

$$h_{SOI} = \alpha\sigma E_0\tau_0 + \hbar v_F\left(-\alpha Q_\perp \tau_x + Q_\parallel \tau_y\right)$$

- Diagonal term

$$E_0(meV) \approx -\frac{0.135\cos(3\theta)}{R(nm)}$$

chiral angle

- Momentum shift

$$Q_\perp\left(nm^{-1}\right) \approx \frac{0.011\cos(3\theta)}{[R(nm)]^2} \qquad Q_\parallel\left(nm^{-1}\right) \approx \frac{0.045\sin(3\theta)}{[R(nm)]^2}$$

Dispersion relation close to Dirac point:

$$E_{\pm,\alpha,\sigma}(k) = \alpha\sigma E_0 \pm \hbar v_F \sqrt{\left(k + \alpha Q_{\parallel}\right)^2 + Q_{\perp}^2}$$

- Kramers degeneracy: $E_{\pm,-\alpha,-\sigma}(-k) = E_{\pm,\alpha,\sigma}(k)$
- Spin-valley degeneracy (for fixed k) lifted

Linearized dispersion around Fermi level:

- Velocities for right- and left-movers identical
- Kramers: only two different velocities $v_A = v_{K\uparrow} = v_{K'\downarrow}$
- SOI strength encoded in dim.less velocity difference $v_B = v_{K\downarrow} = v_{K'\uparrow}$

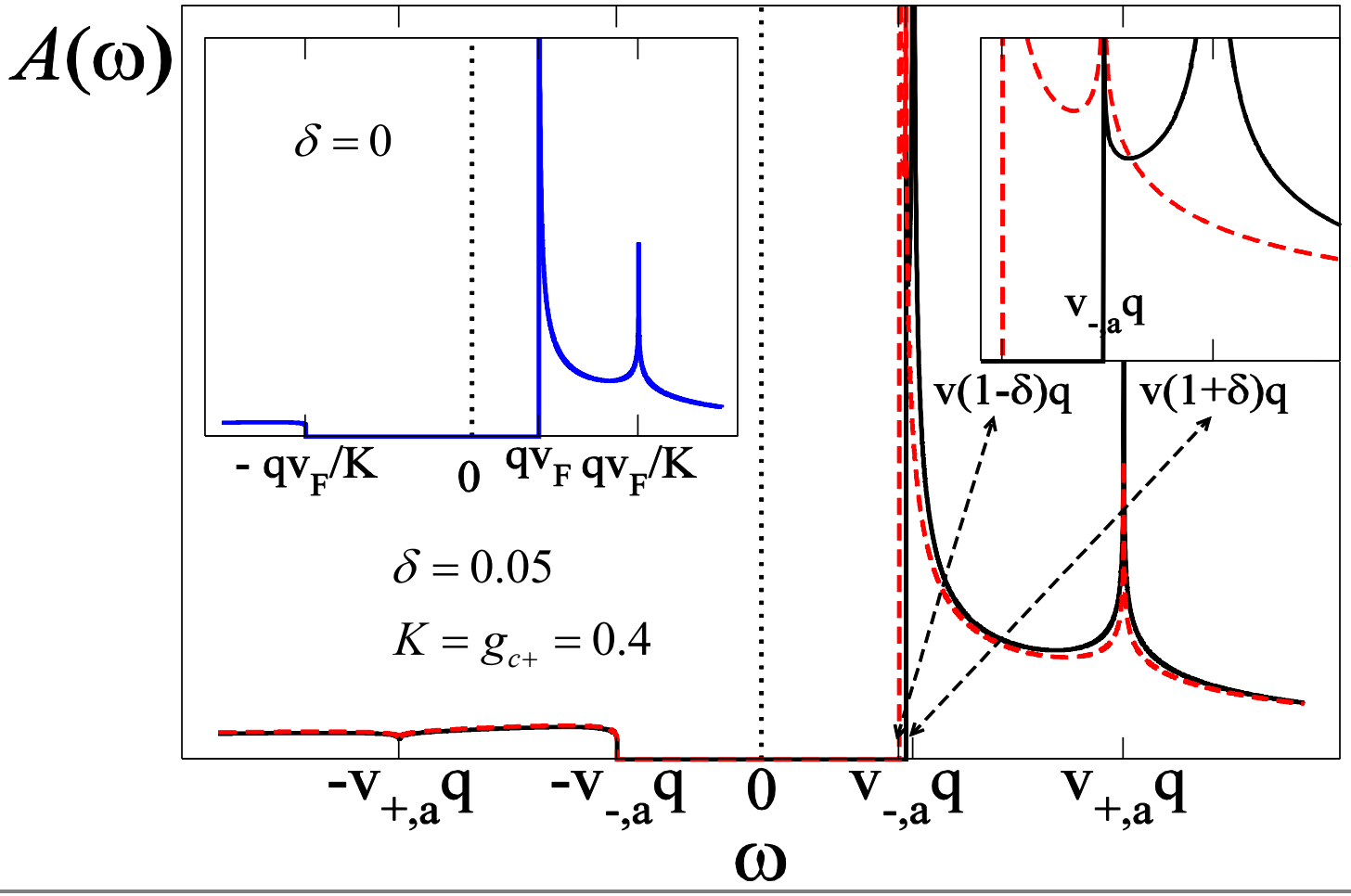
$$\delta = \frac{v_A - v_B}{v_A + v_B} \approx \frac{0.83\cos(3\theta)}{\left[E_F(meV)\right]^2 \left[R(nm)\right]^3}$$

Luttinger liquid with SOI

- Interacting Hamiltonian with SOI can be diagonalized by linear transformation to new boson fields
- SOI only leads to renormalization of the Luttinger liquid parameters g_a, v_a
- Typical values δ≈0.05 : SOI effects on observable exponents (e.g., tunneling density of states) are weak
- Observable effects expected in photoemission spectroscopy

Spectral function

Splitting of power law singularities



Conclusions Part II

- Spin orbit couplings in metallic nanotubes: Luttinger liquid theory still valid, but renormalized velocities and interaction parameters
- Smallness of SOI implies
  - Very weak effect on power-law exponents in typical observables (tunneling density of states)
  - Photoemission spectra are more sensitive: splitting of peak features

A. Schulz, A. De Martino & RE, PRB 82, 033407 (2010)