Title

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Intrinsic and Rashba spin-orbit interactions in graphene sheets

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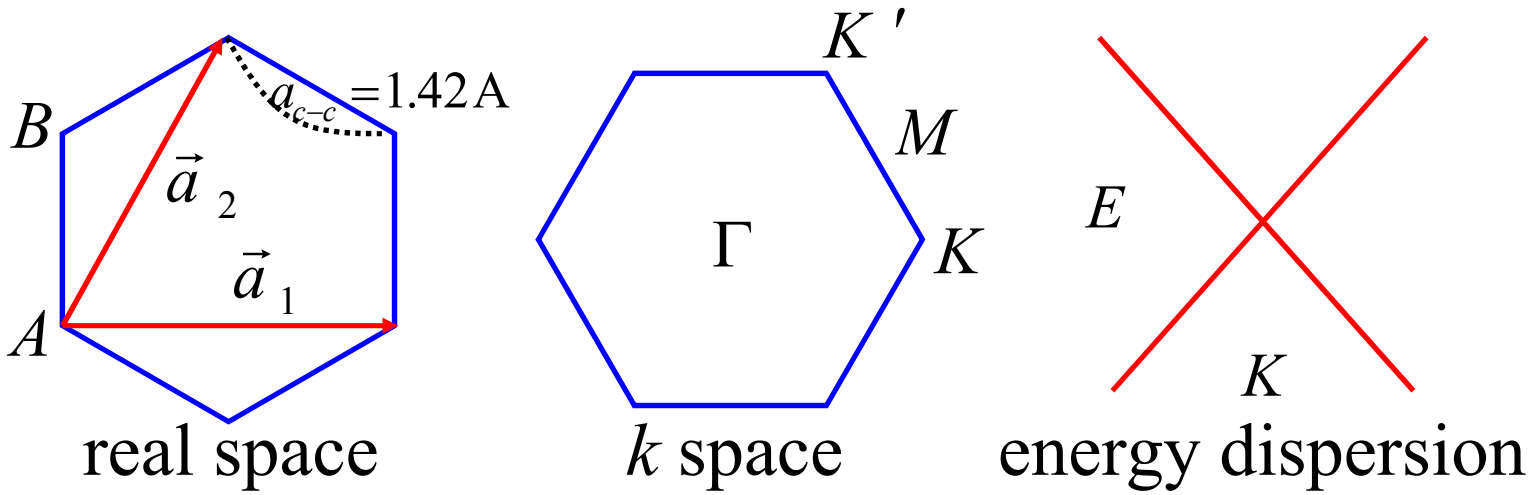
Starting from a microscopic tight-binding model and using second order perturbation theory, we derive explicit expressions for the intrinsic and Rashba spin-orbit interaction induced gaps in the Dirac-like low-energy band structure of an isolated graphene sheet. The Rashba interaction parameter is first order in the atomic carbon spin-orbit coupling strength ξ and first order in the external electric field E perpendicular to the graphene plane, whereas the intrinsic spin-orbit interaction which survives at E is second order in ξ. The spin-orbit terms in the low-energy effective Hamiltonian have the form proposed recently by Kane and Mele. *Ab initio* electronic structure calculations were performed as a partial check on the validity of the tight-binding model.

1. Introduction

1) Graphene

- Graphene is a two-dimensional honeycomb lattice of carbon atoms.
- The energy bands of graphene are described at low energies by a 2D Dirac-like equation with linear dispersion near K/K' in k space.



1. Introduction

2) Extraordinary properties of graphene

- Dirac-like linear dispersion at low energies

$\Rightarrow$ Two-dimensional relativistic electronic system

- Half-quantized quantum Hall effect

$$\sigma_{xy} = -\frac{4e^2}{h}\left(n+\frac{1}{2}\right) \qquad (n=0,1,\ldots)$$

- Quantum spin Hall effect

$\Rightarrow$ A bulk gap with gapless spin filtered edge states

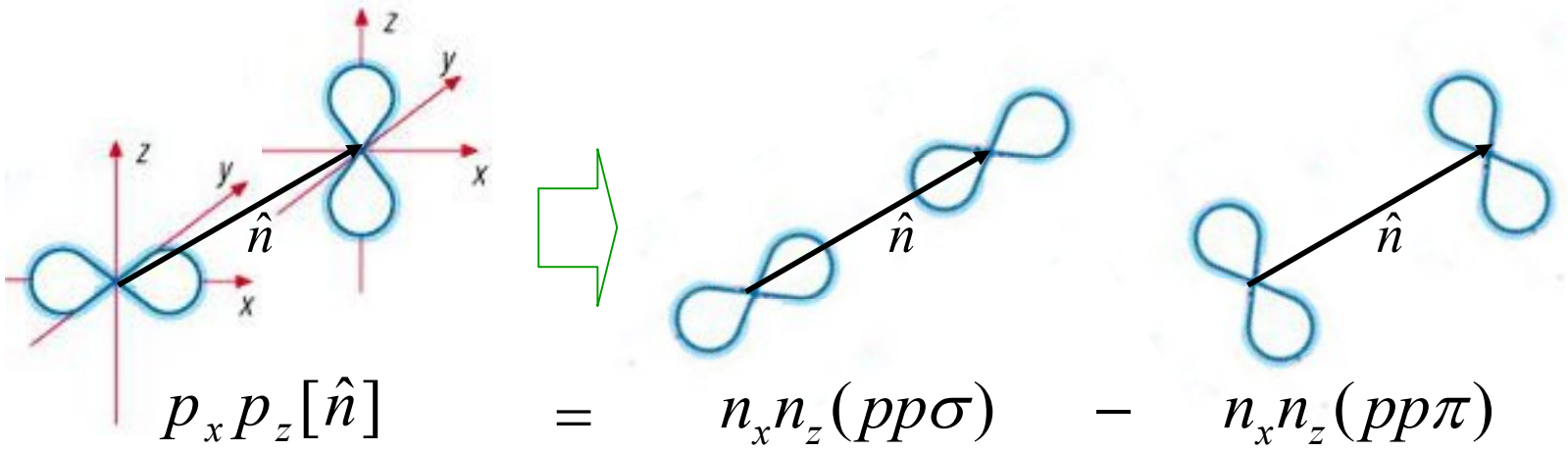
- Excellent mechanical and electronic properties

$\Rightarrow$ Future spintronic devices

2. Tight-binding Model

1) Two-center hopping

- Consider only orbitals on two sites and neglect surrounding orbitals.
- Hamiltonian and overlap matrices can be constructed using a few set of parameters such as $sp\sigma$, $pp\sigma$, $pp\pi$.
- Example



$$p_x p_z[\hat{n}] = n_x n_z(pp\sigma) - n_x n_z(pp\pi)$$

2. Tight-binding Model

2) Atomic spin-orbit interactions

- Approximated by a local atomic contribution.

$$H_{SO} = \xi \sum_i \vec{L}_i \cdot \vec{S}_i$$

3) External gate electric fields

- Approximated by a local atomic Stark-effect term.

$$H_{EF} = eE \sum_i z_i$$

What is the low energy effective model at K and K' in the presence of atomic spin-orbit interactions and external gate electric fields?

3. Perturbation Theory

1) Unperturbed Hamiltonian matrix at K and K'

- Treat spin-orbit and electric fields as a perturbation.

$$H = H_{band} + \Delta H \qquad \Delta H = H_{SO} + H_{EF}$$

- Unperturbed Hamiltonian at K

$\Rightarrow$ Decoupled to (s, p_x, p_y) x (p_z)

$$\alpha = \frac{3}{2}(sp\sigma)\,,\ \beta = \frac{3}{4}[(pp\sigma) - (pp\pi)]$$

	$B\,,\ s$	$B\,,\ p_x$	$B\,,\ p_y$	$B\,,\ p_z$
$A\,,\ s$	0	$i\alpha$	α	0
$A\,,\ p_x$	$-i\alpha$	$-\beta$	$-i\beta$	0
$A\,,\ p_y$	$-\alpha$	$-i\beta$	β	0
$A\,,\ p_z$	0	0	0	0

3. Perturbation Theory

2) Low energy effective Hamiltonian

- *E=0* eigenstates are fourfold degenerate at *K/K'*
- Second-order degenerate perturbation theory

$$H^{(2)}_{mn} = \sum_{l \notin D} \frac{\langle m^{(0)} | \Delta H | l^{(0)} \rangle \langle l^{(0)} | \Delta H | n^{(0)} \rangle}{E_D - E_l^{(0)}}$$

D : degenerate eigenstates

- Effective Hamiltonian matrix at *K*

	$A, p_{z,\uparrow}$	$A, p_{z,\downarrow}$	$B, p_{z,\uparrow}$	$B, p_{z,\downarrow}$
$A, p_{z,\uparrow}$	0	0	0	0
$A, p_{z,\downarrow}$	0	$-2\lambda_{SO}$	$2i\lambda_R$	0
$B, p_{z,\uparrow}$	0	$-2i\lambda_R$	$-2\lambda_{SO}$	0
$B, p_{z,\downarrow}$	0	0	0	0

3. Perturbation Theory

2) Low energy effective Hamiltonian

$\sigma_z = \pm 1$ for A, B
$\tau_z = \pm 1$ for K, K'
$s_z = \pm 1$ for $\uparrow, \downarrow$

- Effective Hamiltonian at K/K'

$$H_{eff} = -\lambda_{SO} + \lambda_{SO}\sigma_z\tau_z s_z + \lambda_R(\sigma_x\tau_z s_y - \sigma_y s_x)$$

- Intrinsic and Rashba spin-orbit coupling

$$\lambda_{SO} = \frac{|s|}{18\,(sp\,\sigma)^2}\xi^2 \qquad \lambda_R = \frac{eEz_0}{3(sp\,\sigma)}\xi$$

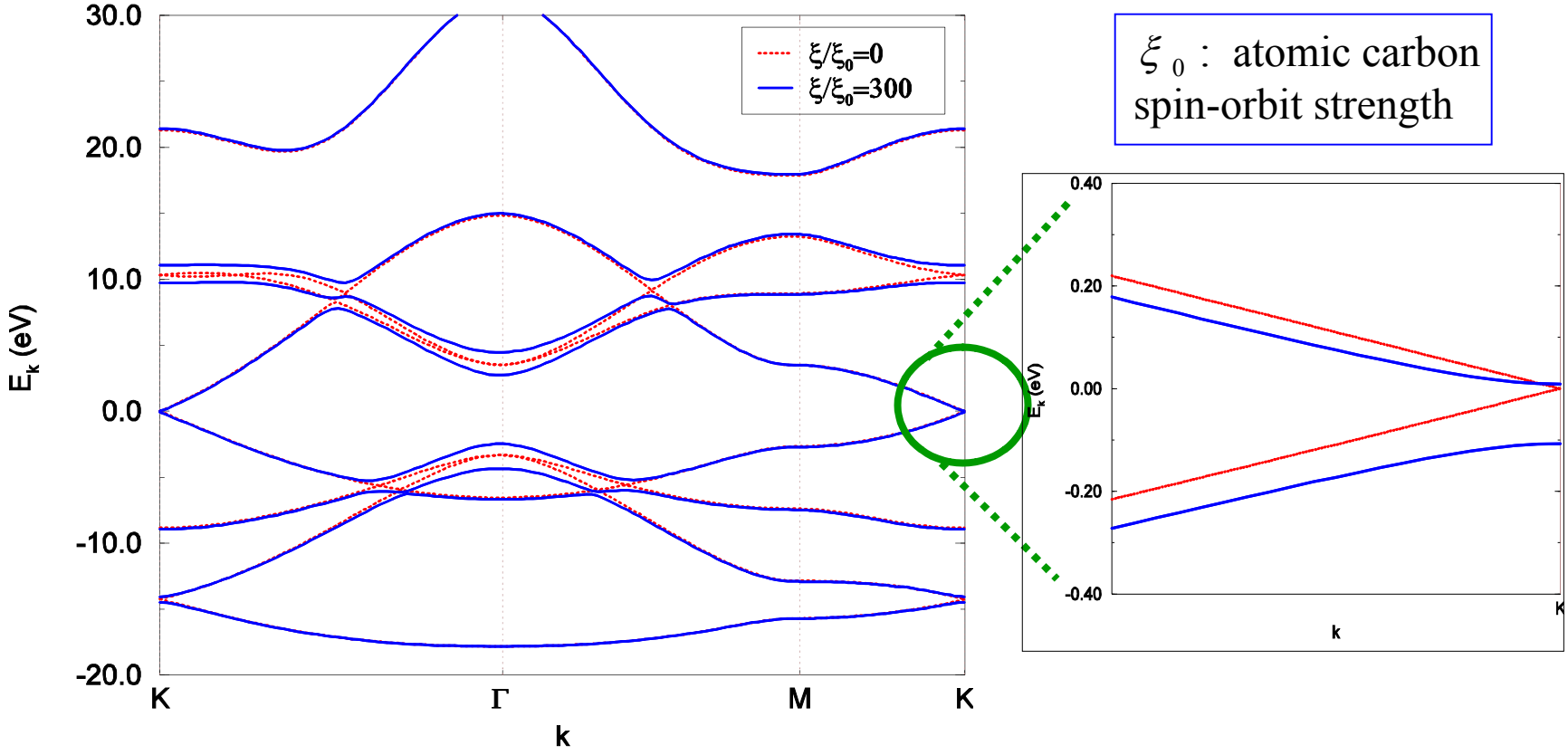
- Energy gap opens when $\lambda_{SO} > \lambda_R$

$$E_{gap} = 2(\lambda_{SO} - \lambda_R)$$

4. *Ab initio* Calculations

1) Band structure in the presence of spin-orbit interactions

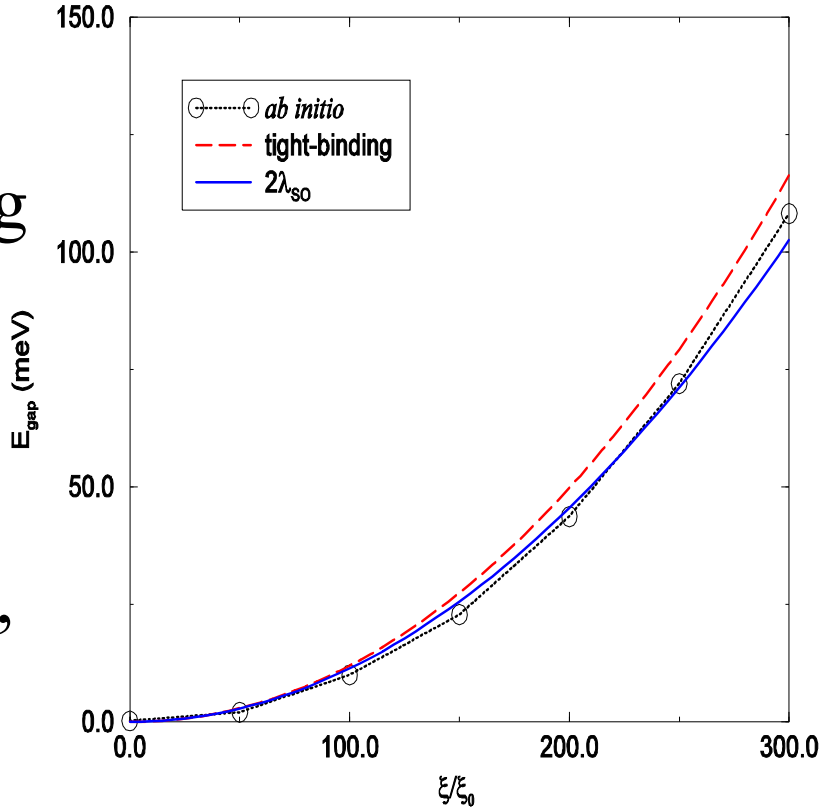
- Tight-binding model with nonorthogonal orbitals



4. *Ab initio* Calculations

2) Energy gap as a function of spin-orbit interactions

- Perform *ab initio* density functional calculations.
- Increase spin-orbit coupling by decreasing the speed of light.
- Energy gaps from *ab initio*, tight-binding and effective model are consistent.



5. Discussion

1) Estimation of coupling constants

- Intrinsic spin-orbit coupling

$$\lambda_{SO} \approx 0.00057\,\text{meV} \approx k_B \times 0.0066\,\text{K}$$

- Rashba spin-orbit coupling with E~50V/300nm

$$\lambda_R \approx 0.00111\,\text{meV} \approx k_B \times 0.129\,\text{K}$$

- Energy gap in the absence of electric fields

$$E_{gap}\Big|_{\lambda_R=0} = 2\lambda_{SO} \approx 0.00114\,\text{meV} \approx k_B \times 0.0132\,\text{K}$$

5. Discussion

2) Implication to quantum spin Hall effects

- Depending on the strength of λ_{SO} and λ_R
  - $\lambda_{SO} > \lambda_R \Rightarrow E_{gap} > 0$, Quantum spin Hall insulator
  - $\lambda_{SO} < \lambda_R \Rightarrow E_{gap} = 0$, Zero gap semiconductor
- In typical experimental condition without disorder $\lambda_{SO} < \lambda_R$, thus quantum spin Hall effect cannot be observed.
- Even in the absence of electric fields, quantum spin Hall effect occurs only below ~0.01K in a clean graphene sample.