Graphene : Spin-Orbit Coupling

EP : Course Seminar

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Intrinsic Spin-Orbit splitting

- Interaction arises due to coupling of internal potential with spin of electrons
- Effective Hamiltonian:

$$H_{SO} = \lambda_I \kappa \sigma_z s_z$$

- Here, s_z : Pauli spin matrix in the electron-spin space
- The dispersion relation for total Hamiltonian $H_0 + H_{SO}$ is

$$\epsilon_\nu = \nu \sqrt{\epsilon_0^2 + \lambda_I^2}$$

- The space inversion and Time reversal symmetries
- Two fold degeneracy in bands

Intrinsic Spin-Orbit splitting

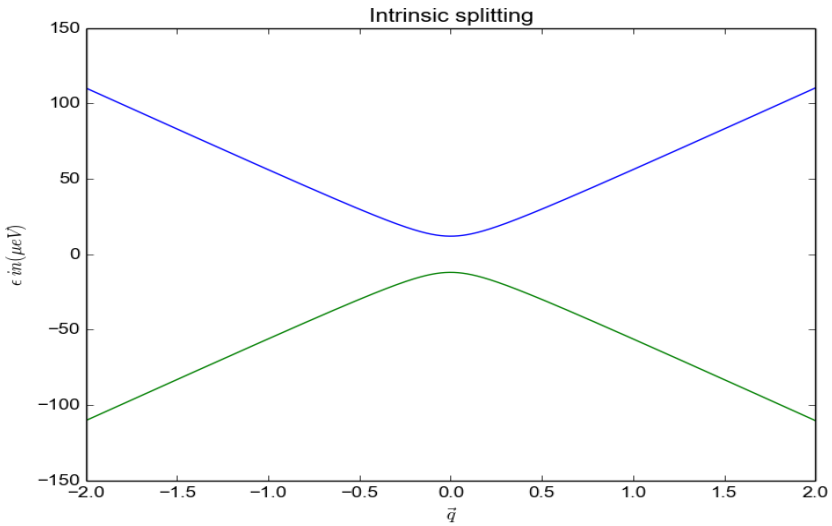

Figure : Intrinsic Spin-orbit splitting

The energy gap of $|2\lambda_I|$ opens at the Dirac points.
Conical shape is replaced by smooth curvature.

Extrinsic Spin-orbit splitting

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- In the presence of transverse electric field,

$$H_{BR} = \lambda_{BR}(\kappa\sigma_x s_y - \sigma_y s_x)$$

- λ_{BR} : Bychkov-Rashba parameter
- The energy-momentum dispersion relation is given by

$$\epsilon_{\mu\nu} = \mu\lambda_{BR} + \nu\sqrt{(\hbar\nu_F k)^2 + (\lambda_{BR} - \mu\lambda_I)^2}$$

- The degeneracy is lifted except at Dirac points
- λ_{BR} depends upon the strength of applied electric field.

$\lambda_{BR} < \lambda_I$

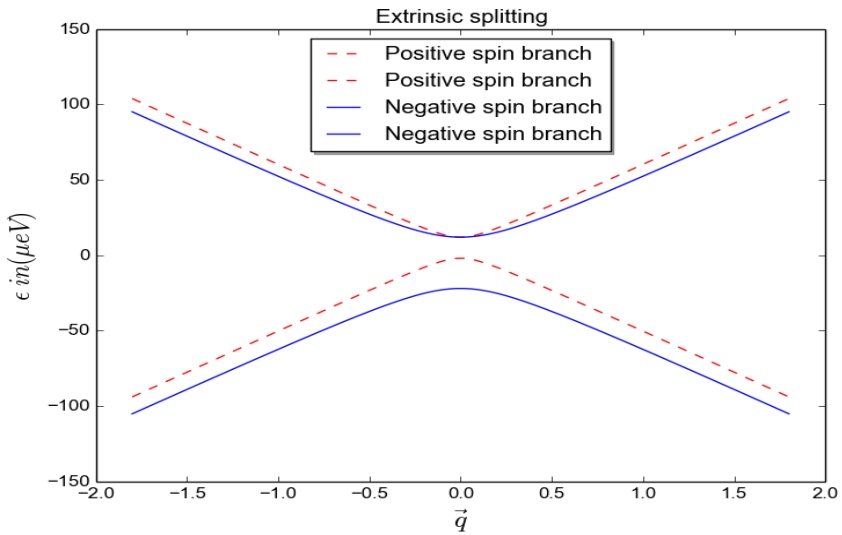

Figure : Extrinsic Spin-orbit splitting when $E = 1.0V/nm$

$\lambda_{BR} = \lambda_I$

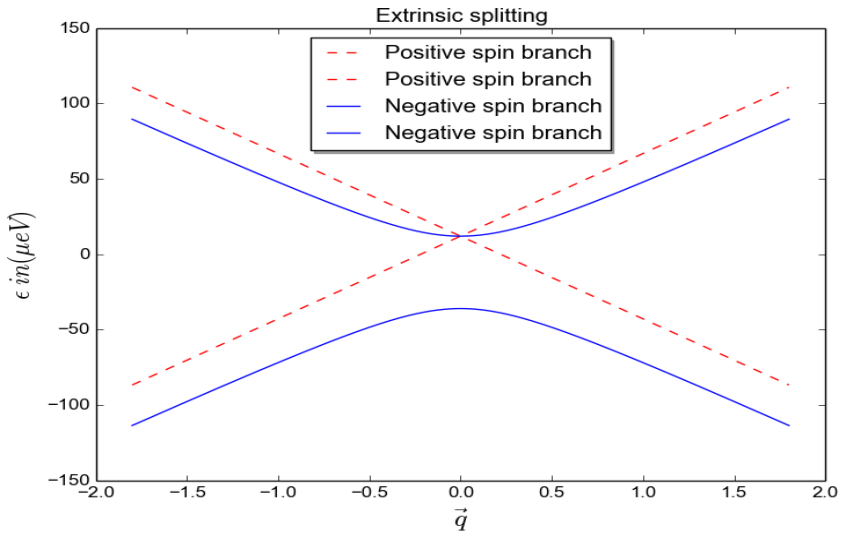

Figure : Extrinsic Spin-orbit splitting when $E = 2.44 V/nm$

- Positive spin branches form massless fermion like cone.
- The remaining branches are massive parabolic bands.

$\lambda_{BR} > \lambda_I$

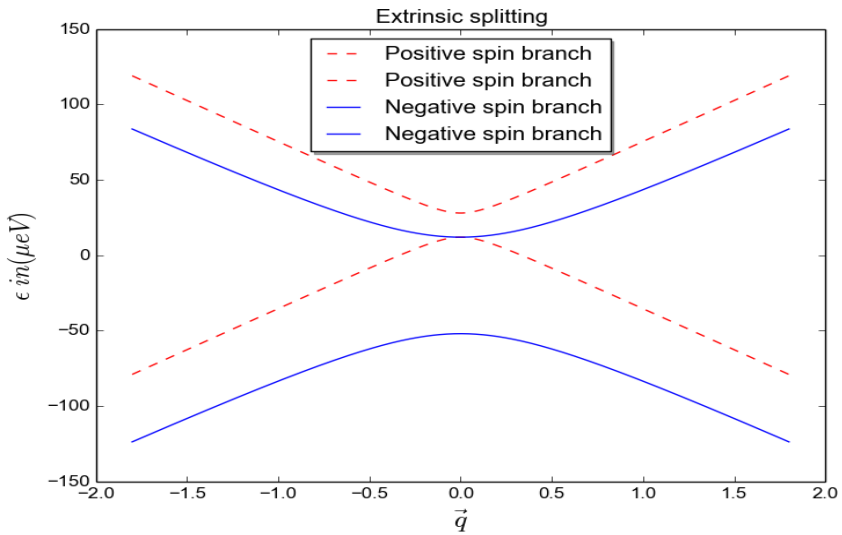

Figure : Extrinsic Spin-orbit splitting when $E = 4V/nm$

Modification in Intrinsic splitting

The authors propose that the value of $2\lambda_I$ is $24\mu eV$. Whereas the earlier reported value is around $1\mu eV$.

- Previous result were not truly from first principle calculations.
- The contribution from d and higher orbitals are also taken into account.
- The contribution from s, p is lower compared to d.
- Removing the contribution of d orbitals gives back the old results.

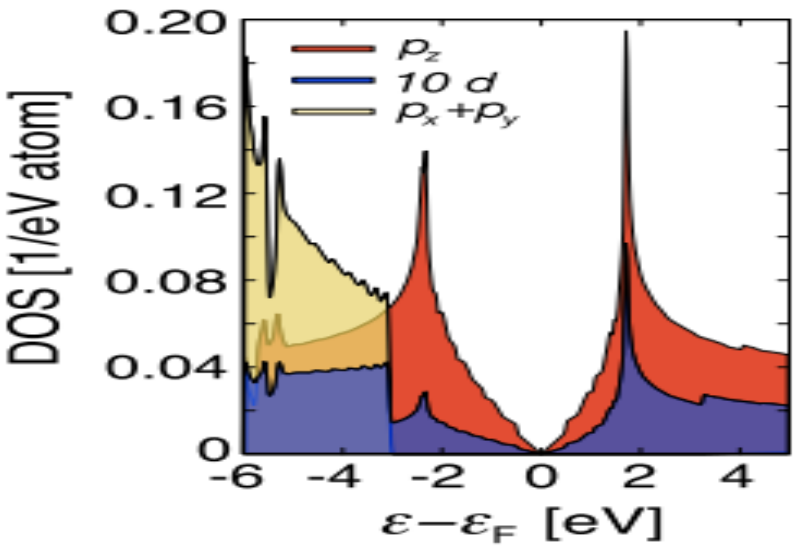

Figure : Projected density of states to particular atomic orbitals

References