Unravelling Spin and Orbital Hall Effects in 2D Materials

Henrique P. Veiga

Supervisor: Professor J. M. Viana Parente Lopes
Co-Supervisor: Professor Aires Ferreira

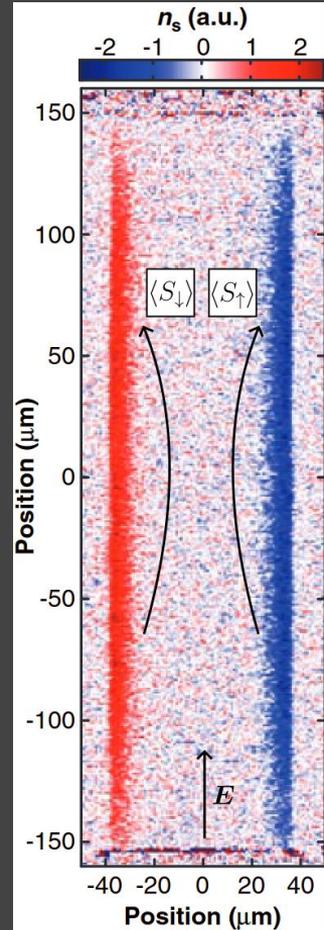# An Overly Executive Summary of this PhD Programme

> **Combine state-of-the-art theoretical and computational methods to understand non-equilibrium phenomena relevant to current efforts in spin-orbitronics**

Bird's-Eye View on Spin and Orbital Transport

❏ Small electric fields generate flow of spin angular momentum (Hirsch, 1999);

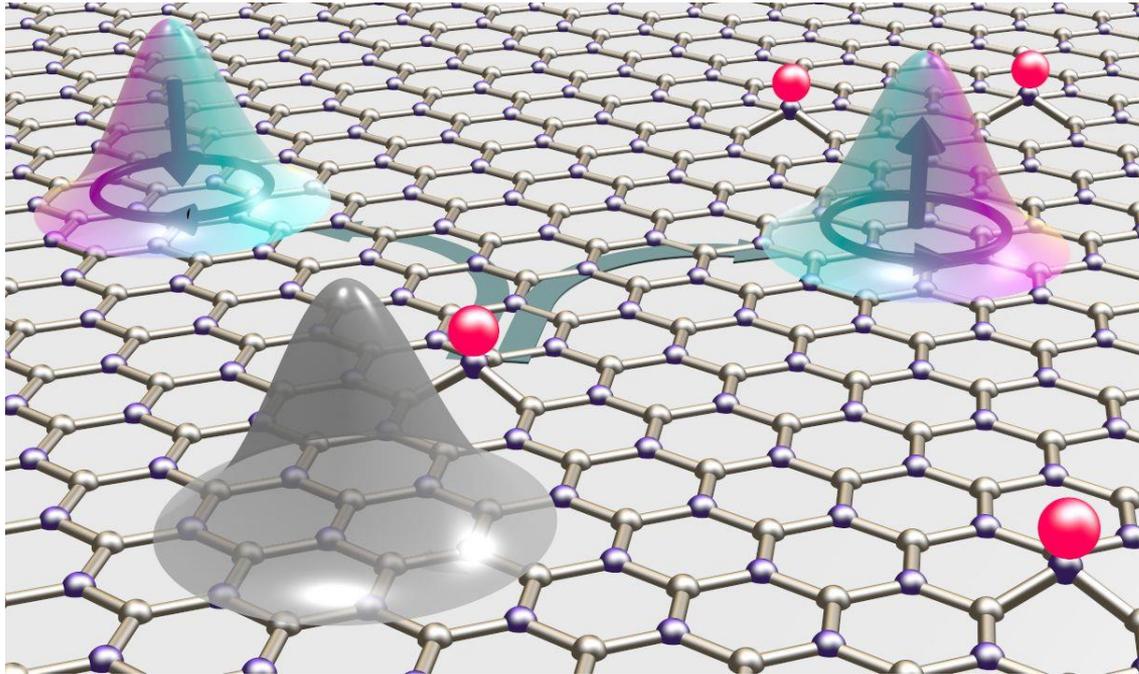<div style="background:black;color:white;text-align:center;">

Spintronics

</div>

❏ Several emergent technologies from the spin Hall effect (SHE) and related transport phenomena;

❏ SHE requires spin-orbit coupling (SOC);

Adapted from (Kato, 2004)

3

Bird's-Eye View on Spin and Orbital Transport

❑ **Early work** (Bernevig, 2005; Go, 2019; Cysne, 2021) **suggest that orbital Hall effects (OHEs) are an appealing alternative to SHE;**
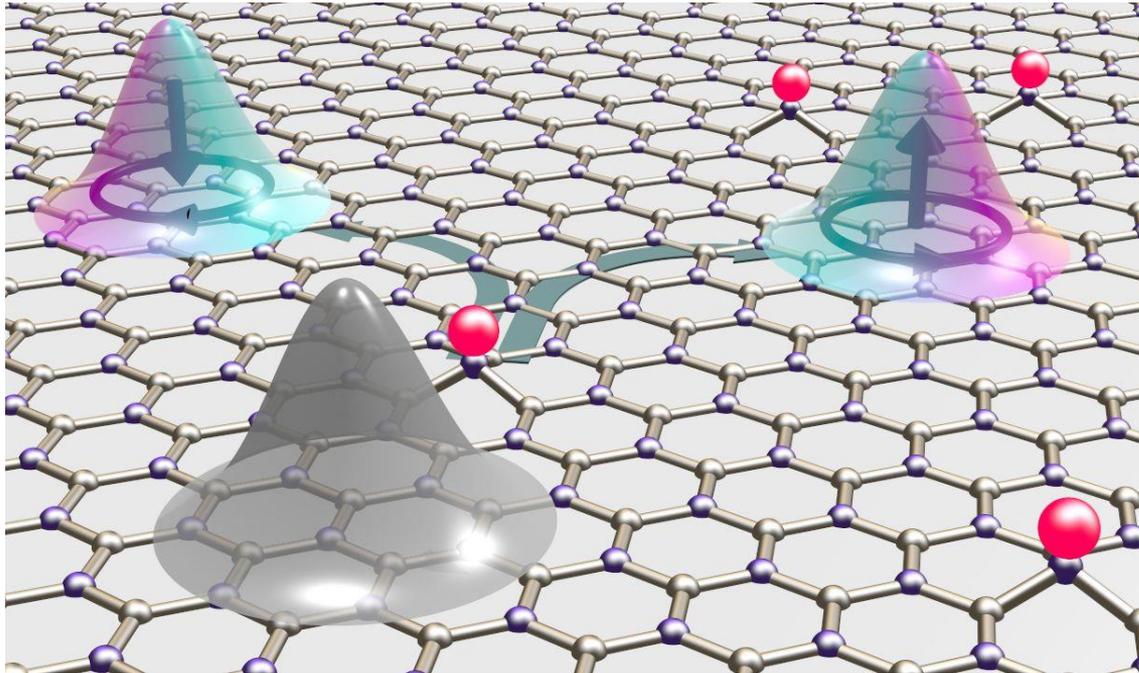

No SOC required
(thus relevant for a large class of materials)

Orbital angular momentum (OAM) plays the role of spin

❑ **Early work** (Bernevig, 2005; Go, 2019; Cysne, 2021) suggest that orbital Hall effects (OHEs) are an appealing alternative to SHE;

No SOC required
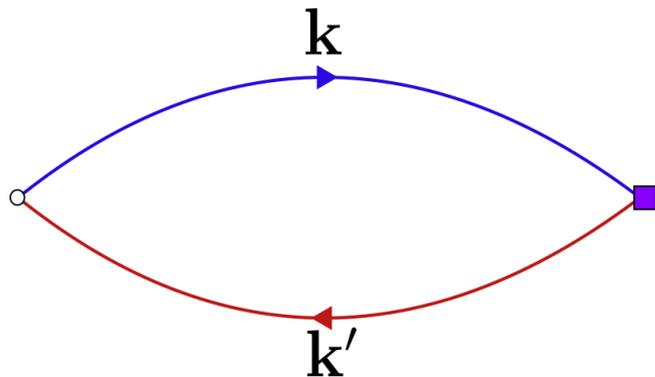(thus relevant for a large class of materials)

Orbital angular momentum (OAM) plays the role of spin

The role of impurity scattering is largely unknown

Twofold Approach

❏ Complementary approach of cutting edge theoretical tools

Momentum-Space Diagrammatics

Real-Space Kernel Polynomial Method

(Covaci, Rappoport, Lopes, Ferreira, 2020)

❏ Resum the complete series of non-crossing diagrams

Diffusive Bulk Response

❏ Develop self-consistent techniques for more realistic disorder landscapes

❏ Construct a microscopic theory of OHE with random dilute impurities

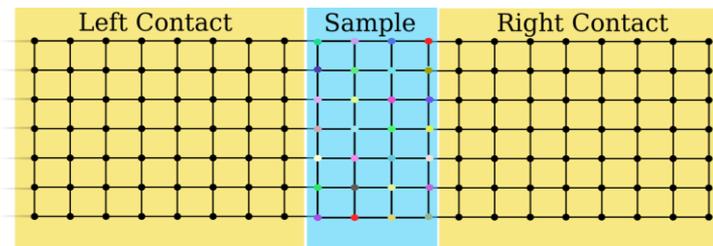Extending the work put forward in (Veneri, 2025)

Twofold Approach

❏ Numerical methods are ideal for fully non–perturbative studies of tight–binding models

❏ Several additions to the KITE source code are planned

Generic linear response functions

Conductance in multi-terminal geometries

$$\mathcal{R}^{ij}_{\alpha\beta}\left(\mathbf{q}, \omega\right) = \frac{\delta\rho^{ij}_{\alpha\beta}(\mathbf{q},\omega)}{E_i}$$

Left Contact   Sample   Right Contact

Twofold Approach

❑ Real-space simulations will be crucial to go beyond the diffusive regime in both SHE and OHE

❑ Nonlocal transport geometries have proven to be essential to observe certain phenomena within SHE (Sheng, 2005; Ren, 2006)

> We expect the same to be important for future studies of the OHE

KITE
quantum transport software

❏ **Clarifying the definition of the Orbital current operator**

❏ **Recent evidence** (Liu, 2025) **indicates that the commonly used recipe to evaluate orbital currents is incomplete at best**

    ❏ Some calculations start from gauge dependent expressions;

    ❏ Ignores intraband matrix elements;

    ❏ More fundamentally, the position operator is ill defined in periodic systems (Marrazzo, 2016);

Numerical methods are ideal to clarify this issue

❏ Nonperturbative by design

❏ Open-boundary conditions

KITE
quantum transport software

❏ Clarifying the definition of the Orbital current operator
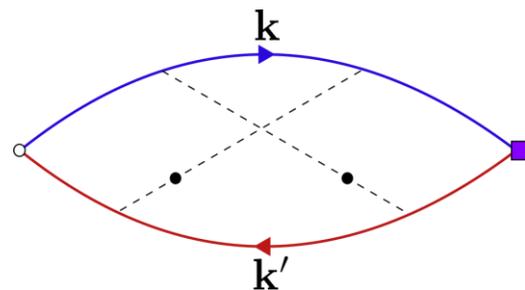
❏ Planned to implement the orbital response function

❏ Tests on simple model systems (e.g. Gapped Graphene, TMDs, …)

❏ Compare preliminary results against literature

❏ Investigate the unphysical discontinuity of the orbital response reported in (Liu, 2024)

❏ Gaussian disorder model;

❏ Evaluation of crossing diagrams (Ado, 2015, Ferreira, 2016);

Work Package
❏ Investigations on the SHE

❏ Study the role of atomic defects and long-range potentials on the SHE
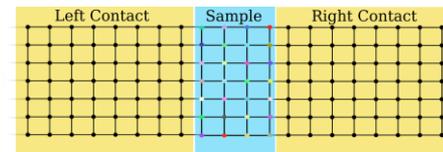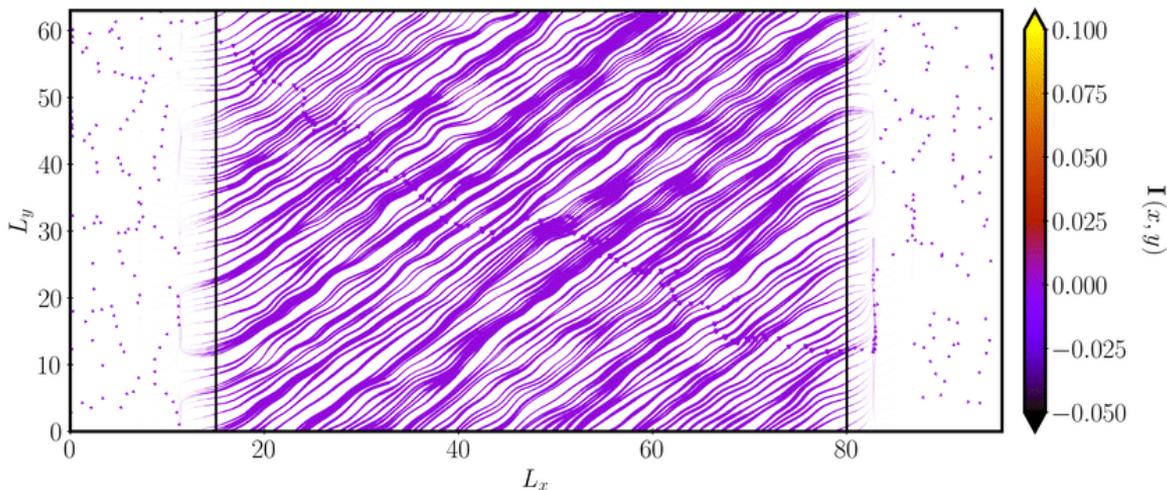
Bulk Conductivity

Multi-terminal Geometry

❏ All evidence for skew-scattering has been theoretical based on momentum space. We wish to provide the first evidence for skew scattering in real-space

❏ Twisting Effects

KITE
quantum transport software

❏ Interplay between orbital and spin Hall effects

❏ Real-space imaging of orbital currents in realistic transport geometries

We expect the knowledge drawn from ongoing projects to be key in shedding light at emergent orbital Hall effects (Gobel, 2024)

Work Package

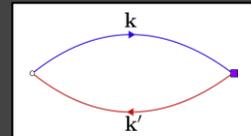❑ Interplay between orbital and spin Hall effects

Unlock the interplay of SHE and OHE

Introduction of Rashba effect

Real-Space orbital Edelstein effect

Generalise (Aires, 2021) and derive a quantum kinetic equation for OHE

First steps to unified theory of spin-orbital dynamics in 2D materials

1. Develop new numerical methods

1. Clarify the proper evaluation of orbital currents

1. Construct a theory of diffusive OHE for 2D semiconductors

1. Perform real–space studies of OHE and SHE

1. Unveil the interplay between orbital and spin Hall effects

Research Project's Goals

1. Develop new numerical methods

1. Clarify the proper evaluation of orbital currents

1. Construct a theory of diffusive OHE for 2D semiconductors

1. Perform real-space studies of OHE and SHE

1. Unveil the interplay between orbital and spin Hall effects

Research Project's Goals

1. Develop new numerical methods

1. Clarify the proper evaluation of orbital currents

1. Construct a theory of diffusive OHE for 2D semiconductors

1. Perform real–space studies of OHE and SHE

1. Unveil the interplay between orbital and spin Hall effects

Research Project's Goals

1. Develop new numerical methods

1. Clarify the proper evaluation of orbital currents

1. Construct a theory of diffusive OHE for 2D semiconductors

1. Perform real-space studies of OHE and SHE

1. Unveil the interplay between orbital and spin Hall effects

Research Project's Goals

1. Develop new numerical methods

1. Clarify the proper evaluation of orbital currents

1. Construct a theory of diffusive OHE for 2D semiconductors

1. Perform real-space studies of OHE and SHE

1. Unveil the interplay between orbital and spin Hall effects