# Wave Packet Dynamical Simulation of Magnetic Effects in 2D Materials

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Two dimensional (2D) materials and 2D heterostructures have extraordinary physical properties, determined both by the pristine crystal lattice and its defects. Understanding the effect of magnetic fields on the electronic structure and transport properties of these materials is important for several reasons: (1) magnetic fields arising near magnetic defects, (2) pseudo-magnetic fields [1] arising because of structural defects, and (3) one-dimensional (1D) defects (edges and 2D grain boundaries), where magnetic and topological phenomena may occur. We studied such effects utilizing two calculation methods based on wave packet (WP) dynamics. (1) We model the atomic- and electronic structure of the perfect 2D lattice by a local atomic pseudopotential [2] and calculate the time dependent scattering [3] of a Bloch WP on the defect represented by a scalar potential. (2) We describe the perfect crystal by a dispersion relation derived from band structure calculation [4] and study the scattering of a WP on a vector potential corresponding to the pseudo magnetic field of the defect. The model calculations were performed on a graphene sheet but the second method is applicable for any 2D material where electronic structure calculations are available.

## References

[1] P. Kun et al, 2D Mat. Appl. 3 (2019) 11.
[2] A. Mayer, Carbon 42 (2004) 2057.
[3] G. I. Márk et al, Phys. Rev. B 85 (2012) 125443.
[4] P. Vancsó et al, Appl. Sci. 11 (2021) 4730.

## Figures

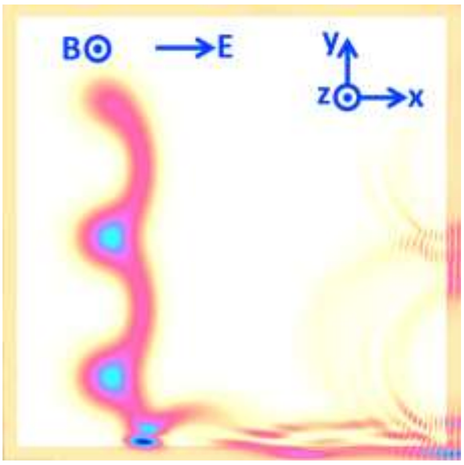


**Figure 1:** Wave packet scattering on a topological insulator model. The time integrated probability density of the wave packet propagating in perpendicular electric- and magnetic fields demonstrates that there is no conduction in the bulk but conduction occurs at the boundary.