2D Materials in Strong Magnetic Fields: Hofstadter physics from first-principles

Vasil Rokaj [1,*], Markus Penz[1], Michael Sentef[1], Michael Ruggenthaler[1], and Angel Rubio[1]

[1] *Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany*
[*] *vasil.rokaj@mpsd.mpg.de*

July 2, 2020

We present a first-principles approach for treating 2D materials from weak to strong magnetic fields [1] and more precisely from the integer to the fractal quantum Hall regime. Our approach relies on the expansion on a correlated basis consisting of Landau levels and Bloch waves. In this manner we are able to compute energy bands of 2D materials as a function of the magnetic field strength and to capture the fractal spectrum of the Hofstadter butterfly [2] from first-principles. Further, the connection of the fractal spectrum to experimental transport measurements [3] will be presented, and how our theory allows for the explanation of these measurements and the intricate phenomena related to the Hofstadter butterfly.

References

[1] Vasil Rokaj, Markus Penz, Michael A. Sentef, Michael Ruggenthaler, and Angel Rubio. Quantum electrodynamical bloch theory with homogeneous magnetic fields. *Phys. Rev. Lett.*, 123:047202, Jul 2019.

[2] Douglas R. Hofstadter. Energy levels and wave functions of bloch electrons in rational and irrational magnetic fields. *Phys. Rev. B*, 14:2239–2249, Sep 1976.

[3] Lei Wang, Yuanda Gao, Bo Wen, Zheng Han, Takashi Taniguchi, Kenji Watanabe, Mikito Koshino, James Hone, and Cory R. Dean. Evidence for a fractional fractal quantum hall effect in graphene superlattices. *Science*, 350(6265):1231–1234, 2015.