Nano-bubbles within a suspended bilayer graphene

In recent years 2D materials have become one of the most studied systems within physics due to a whole array of exotic properties that these materials exhibit. The 2D nature of these systems has made it possible to apply strain, stretching it in all possible ways (like an elastic piece of paper) in what is now a new field in physics called ‘straintronics’. Many exotic properties can emerge from straining such as pseudo-Landau levels [2] and highly correlated electron states such as superconductivity and Mott insulation. The application of strain can be achieved in several ways such as the combination of materials into van der Waals heterostructures, mechanically applied strain and the use of gas-induced pressure. This last one can be used to create nano-scale bubbles by trapping gas between a bulk substrate and a 2D material of choice. Instead of a bulk substrate, this can also be done for a bilayer graphene, creating a region where a “nano-sphere” of noble gas exists between the bilayer graphene that exhibits enormous amounts of strain, locally altering the electronic properties. Using molecular dynamics this can be simulated at low temperatures using LAMMPS [1]. We would be able to see the transition from a strained monolayer graphene within the bubble to unstrained bilayer graphene in the bulk. Further possibilities are the introduction of a periodic lattice and the application of an electric gate which could possibly tune the emergence of Landau levels by inducing a height dependent potential gradient [3,4]. In order to calculate this, you will have to create your very own model and calculate the electronic properties by using state-of-the-art software such as Pybinding (Python) [5] and KITE [6].

[1] https://www.lammps.org

[2] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. **81**, 109 (2009)

[3] E. V. Castro, M. A. Cazalilla, and M. A. H. Vozmediano, Phys. Rev. B **96**, 241405(R) (2017)

[4] V. Lukose, R. Shankar, G. Baskaran, Phys. Rev. Lett. **98**, 116802 (2007)

[5] https://docs.pybinding.site/en/stable/

[6] https://quantum-kite.com