Quantum Transport in Nanoporous Graphene

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Abstract: Abstract...

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Project Repository: https://github.com/rwiuff/QuantumTransport

A. Intro

B. πorbitals and Basis sets

The main scope of this paper is dealing with electron transport in novel nanoporous graphene devices. When modeling such transport one needs to adress the orbital structure of carbon lattices and later this will motivate the use of tight-binding and Green's functions. In its basic form graphene can be devided into rings of carbon atoms as shown in Fig. 1. In the (x, y)-plane the carbon atoms are bound in sp^2 orbitals as shown in Fig. 2.

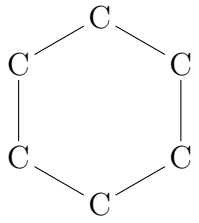

Figure 1: *Graphene lattices consists of hexagonal arrangements of carbon atoms.*

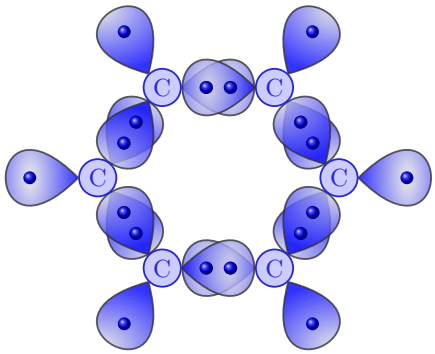

Figure 2: *Carbon atoms in a hexagonal lattice are sp^2 hybradised in the (x, y)-plane.*

This hybradisation lock all but one valence electron for the carbon atoms. These electrons exists in a p-orbital in the z-direction. Fig. 3 shows the valence orbitals of carbon.

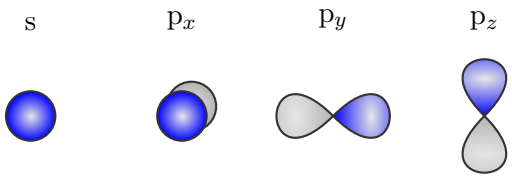

Figure 3: *The valence orbitals of carbon.*

The last electron in the p_z orbital does not mix with the tightly bound s, p_x and p_y electrons and moves more freely. The p_z orbital is also known as the π-orbital and as such the electron inhibiting is called a π-electron. Through a carbon lattice the π-electrons will travel through π-orbitals, switching sign as they go as shown in Fig. 4.

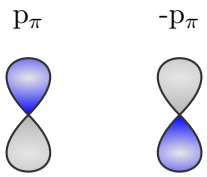

Figure 4: *When going from one carbon atom to another, the π-electron goes betwenn p_π and $-p_\pi$.*

[1]

ACKNOWLEDGMENTS

The authors would like to thank...

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[1] G. Calogero, N. R. Papior, B. Kretz, A. Garcia-Lekue, T. Frederiksen, and M. Brandbyge, Electron Transport in Nanoporous Graphene: Probing the Talbot Effect, Nano Letters **19**, 576 (2019).

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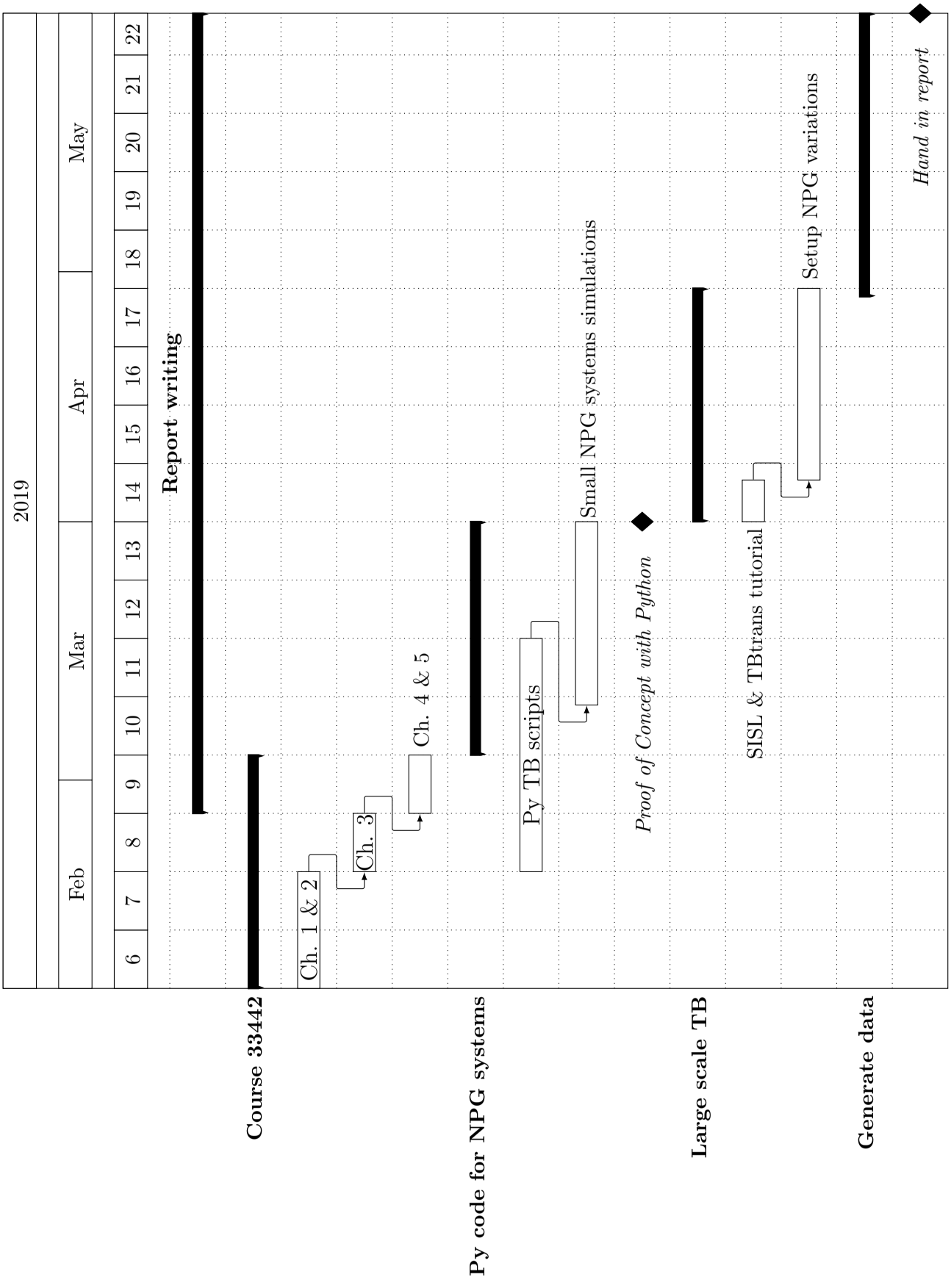
Appendix A: Project overview

A Gantt chart is provided on the next page.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