

Accelerating modeling of Bernal-stacked bilayer graphene devices: effective four-band model

A. Mreńca-Kolasińska¹, S.-C. Chen² and M.-H. Liu³

¹*AGH University, Faculty of Physics and Applied Computer Science, Cracow, Poland*

²*National Formosa University, Department of Electro-Optical Engineering, Yunlin, Taiwan*

³*National Cheng Kung University, Department of Physics, Tainan, Taiwan*

alina.mrenca@fis.agh.edu.pl

Bernal-stacked bilayer graphene (BLG) is a versatile platform for a variety of electronic devices, thanks to its electrostatically tunable band gap. Modeling of quantum transport and other phenomena in BLG has been typically done within the atomistic tight-binding model. However, for realistic, micrometer scale devices it is extremely demanding due to the high computational burden, and thus, it has remained limited to quasi-1D systems.

The main focus of this work is the development of the effective square lattice model, based on the continuum Hamiltonian of BLG. We demonstrate its performance for transport modeling within the Landauer-Büttiker formalism by revisiting recent experiments on BLG devices. In particular, we consider phenomena typical for Bernal-stacked bilayer graphene: transition from Klein to Anti-Klein tunneling [1] and Aharonov-Bohm effect in gate-defined quantum ring [2]. The model can capture the experimental result well, providing a reliable and fast way to model large-scale systems. It can be particularly useful for revealing physical phenomena in systems including BLG-based superlattices, quantum dots, and quantum point contacts.

References

[1] R. Du *et al.*, Phys. Rev. Lett. 121, 127706 (2018).

[2] S. Iwakiri *et al.*, Nano Lett. 22, 6292 (2022).

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