Spin transport in edge-disordered graphene nanoribbons using machine learning

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Graphene nanoribbons (GNRs) have emerged as particularly attractive building blocks for nanodevices. At the nanoscopic scale, geometrical effects can critically affect electronic, magnetic, and transport properties. For example, zigzag-edged graphene nanoribbons (ZGNRs) can display spin-polarized edge states, which have very promising applications in future spintronics [1,2]. Despite impressive advances in fabrication techniques, it is an ongoing challenge to produce and control the desired transport properties in GNR devices. Therefore, characterising the effects of realistic disorders on device behaviour remains crucially important.

Theoretical predictions of spin properties, usually calculated using a time-consuming self-consistent (SC) procedure, can be intractable in computational resources required to deal with realistic system size. Machine learning (ML) techniques have been employed in various fields, such as consumer recommendation systems, protein folding and chemistry [3], to exploit patterns in data and make predictions. In this work, we address ML techniques to accurately estimate the magnetic moment profiles for arbitrarily large and disordered systems. Alongside conventional techniques, developing a neural network tool that accurately estimates the magnetic profile for large and disordered GNRs, we have conducted a thorough analysis on how the edge disorder impacts the robustness of spin-currents in GNRs. The robustness of spin-currents in ZGNRs is highly intertwined with the edge roughness profile at low energies. Whereas spin current is persistent in smooth-edged ribbons due to the absence of back-scattering possibilities, short-ranged scatterers in rough-edged profiles curtail the establishment of edge spin-polarised currents. Our results highlight how ML, by predicting quickly and accurately moment profiles for realistic systems, complements conventional transport techniques to study magnetism and spin transport in 2D materials.

References

[1] Fujita et al., J. Phys. Soc. Jpn. 65, 1920–1923 (1996)
[2] Son Y. et al., *Nature* 444, 347–349 (2006)
[3] Rupp M., IJQC, 115.10.1002/qua.24954. (2015)

Figures

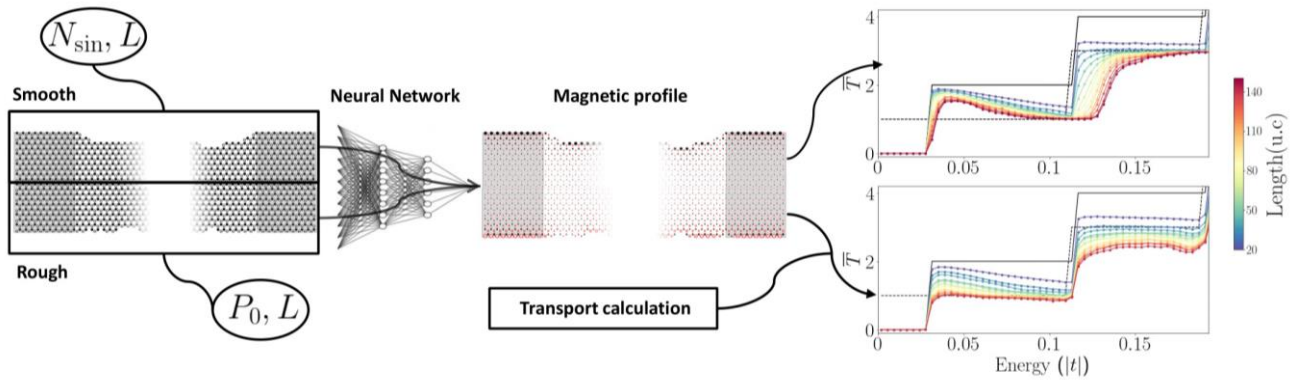

Figure 1: Workflow for the study of spin transport on disordered ribbons. We start by generating a large amount of configurations with different disorder profiles. The previously trained NN then accurately predicts the magnetic profile of the ribbons. This information allows to obtain the spin-polarised transmissions and to state the average behaviours of spin-currents according to the disorder profile.