Machine learning description of spin transport in disordered graphene nanoribbons

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Graphene and other 2D materials could play crucial roles in future nanodevices. At nanoscopic scales, 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 spintronic applications [1,2]. However, disorder in the lattice structure, particularly near edges, is extremely difficult to eliminate, and can lead to substantial changes in the properties of these systems. Therefore, characterising the effects of realistic disorders on device behaviour remains crucially important.

Theoretical predictions of spin properties, usually calculated using time-consuming self-consistent (SC) procedure, can be computationally demanding for realistic system sizes. 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 employ ML techniques to accurately estimate the magnetic moment profiles for arbitrarily large and disordered systems. Alongside conventional techniques, this allows us to investigate in detail the effect of edge disorder on spin transport in graphene nanoribbons at realistic scales.

The robustness of spin-currents in ZGNRs is highly intertwined with the edge roughness profiles. Whereas a spin current can persist in smooth-edged ribbons due to a suppression of back-scattering, short-ranged scatterers in rough-edged profiles curtail the establishment of edge spin-polarised currents.

Our results highlight how ML techniques, by predicting quickly and accurately moment profiles for realistic systems, complement conventional transport methods in the study of magnetism and spin transport in 2D materials.

References

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[3] Rupp M., IJQC, 115.10.1002/qua.24954. (2015)

Figures

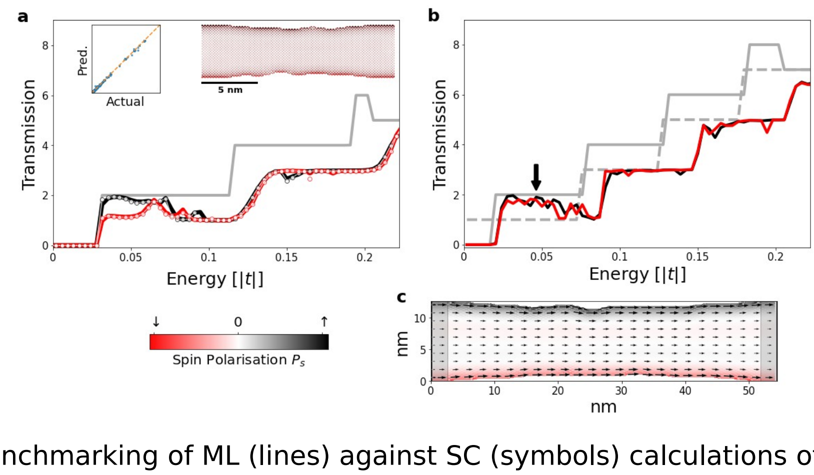

Figure 1: a- Benchmarking of ML (lines) against SC (symbols) calculations of spin-dependent transmission for a 7-nm wide system. The left inset shows the accuracy of the moment prediction and the right inset shows the moment profile.
b- Once trained, the spin-related transmission for a much larger system (shown in **c**)is obtained.
c- A map of local currents and spin-polarisation for the system in **b.**