

Bubbles and perforations in graphene using a patched Green's function technique

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We present a new approach to the widely used recursive Green's function technique and its application to local electronic and transport calculations of graphene nanostructures such as bubbles and perforations.

First, we consider strained graphene bubbles and calculate the local density of states (LDOS) directly from tight binding thus going beyond the effective Dirac model. We demonstrate how the LDOS in nanobubbles with clamped edges contains strong signatures of this edge. In particular, we show how the clamped edge gives rise to significant Friedel type oscillations and spatial variations in the LDOS, as shown in Fig. 1a. The Friedel effects mix with any pseudomagnetic effects arising from the strain field. As many attempts to reliably produce nanobubbles result in significant edge effects, it is important to note that, when looking at the LDOS, simple size dependent features can become comparable to the effect of the strain induced pseudomagnetic field.

Secondly, we consider the transmission between two point probes connected to an extended graphene sample. This demonstrates how the patched Green's function technique efficiently calculates transport properties for widely separated features while still allowing for local mapping of bond currents and LDOS. Specifically, we show the current flow around perforations of the graphene lattice. Here localised states around zigzag edge segments of the perforation give rise to distinct signatures in the transmission spectrum. Furthermore, local mapping of the bond currents show how the transmission signatures are connected to vortex like current paths formed near these edges, see Fig. 1b.

The developed method is based on Green's functions and considers several device patches described by the Hamiltonian, H_D , and connected through a self energy, Σ_B , describing the extended part of the system as shown schematically on Fig. 1c. The patched Green's function technique thus allows for calculations of non-periodic structures embedded within extended samples. The calculation scheme relies on a combination of analytic expressions for infinite pristine systems and an adaptive recursive Green's function scheme. The combination allows us to efficiently calculate both local electronic and transport properties while including multiple leads on arbitrary geometries within extended samples.

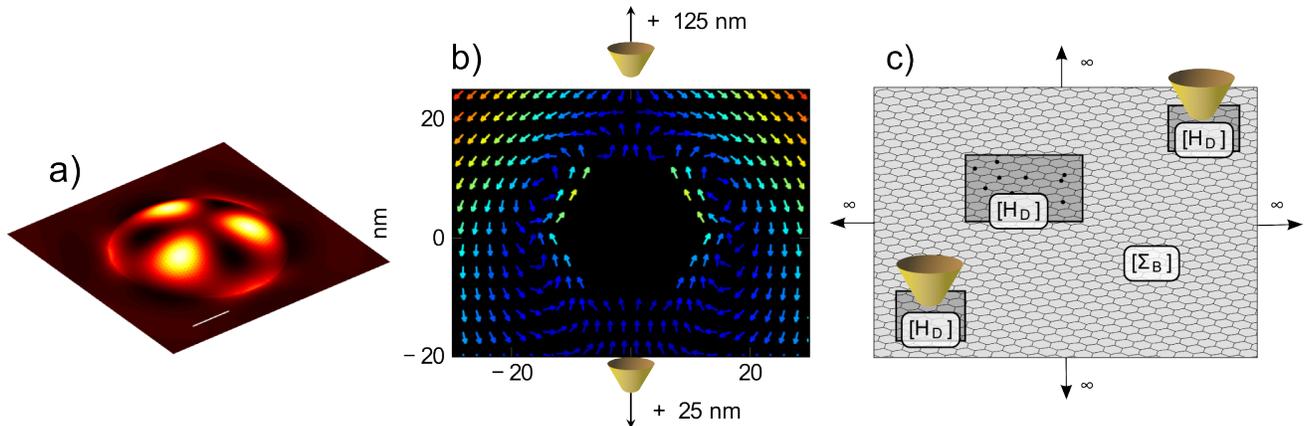


Fig. 1: **a)** Shows deformation profile of a graphene bubble. The colormap indicates the difference in LDOS between the situation with and without the bubble. Yellow indicates high LDOS difference and black denote zero difference. The scalebar is 5 nm. **b)** The arrows indicate the bond currents emitted from the top probe and passing a perforation with zigzag edges (region without arrows). The color of the arrows correspond to the size of the current. **c)** Schematic of the patched Green's function calculation setup. Where the device is indicated in dark gray and the extended part, described efficiently by the self energy Σ_B , is indicated by light gray.