Theory of dual probes on graphene structures

This thesis concerns the development of theoretical and computational methods for multiprobe systems and their application to nanostructured graphene. Recent experimental advances emphasize the usefulness of multi-probe techniques when analyzing the electrical properties of nanoscale samples. The multi-probe setup, however, is conceptually different from the standard calculation setups which either disregard the effects of the probes altogether or use probes connected at the edge of a finite device region. In the multi-probe setup, on the other hand, the device region is infinite and extends all around the local probes. This necessitates a reformulation of the conventional calculation methods allowing for the description of non-periodic structures embedded within infinite samples.

The two-dimensional material graphene, is a highly interesting system for multi-probe characterization as graphene is purely surface and exhibits a wide range of highly intriguing electronic properties. Using a dual probe setup, we demonstrate the application of the developed formalism to a number of different graphene-based systems. The conductance between the two probes in either scanning or spectroscopy mode, shows quantum interference patterns around impurities or crystalline edges. These interferences can be used to reveal important information about the scattering processes taking place. The thesis furthermore discusses nanostructuring such as perforations or local gating. We show how single states or modes and their interplay gives rise to resonances in the dual probe conductance and can be associated with vortex-like current patterns either guiding or suppressing the current.

We further address the effect of strain in graphene when subjected to mechanical deformations giving rise to so-called pseudomagnetic fields. Here we investigate strained graphene bubbles ("pseudomagnetic dots") directly from tight binding, effectively going beyond the Dirac approximation. In this way, we study the local density of states of different pseudomagnetic dots in real space and show Friedel-type oscillations caused by the finite size of the dots, sublattice polarization and Landau quantization. Additionally, we use the dual probe conductance to demonstrate the current guiding ability of the pseudomagnetic fields leading to preferential scattering directions responsible for the observed pseudomagnetic focusing and anti-focusing effects.

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