Quantum Transport in two-dimensional Systems

Artificial Intelligence applied to Material Science

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The control of electronic transport through nanostructures is a research domain of great fundamental interest. It is also crucial for the development of modern electronic devices. While the ongoing miniaturization of electronic devices leads to an increasing importance of quantum effects, it simultaneously enhances the sensitivity of the transport properties with respect to material imperfections like crystal defects, random dopant positions, etc. Such imperfections lead to an uncontrolled disorder configuration that varies from one sample to another. As a consequence, the transport properties of the sample fluctuate even though all experimental control parameters are identical.

In this project, we will make a first step towards a complete microscopic characterization of twodimensional materials, including the microscopic disorder configuration of a sample. To this end, we will investigate the dependence spatially resolved quantum transport of properties on the disorder configuration of the sample. The Scanning Gate Microscopy (SGM) response [1,2], which is the measured



conductance change as a function of the position of a local potential perturbation created by a charged AFM tip scanning the surface of a sample, could be well suited for such a study. While it is possible to calculate the SGM response of two-dimensional electron gases in quantum materials like semiconductor heterostructures, graphene, or transition metal dichalcogenide (TMD) monolayers for a given disorder configuration [3,4,5] (the figure shows an example for the system of Ref. [5]), no method is known that allows to solve the inverse problem, that is to determine the disorder configuration from the SGM response.

We will investigate whether Artificial Intelligence (AI) methods allow to determine features of the underlying disorder potential from the SGM response. A possible route towards such a material characterization method is as follows. First, one calculates the SGM response for many microscopically different random disorder configurations of a two-dimensional electron system in a quantum material with simple sample geometry. Second, the resulting set of data is used to train an appropriately sized neural network, that might recognize data patterns and thereby become able to identify features of the disorder configuration arising from SGM data.

The theoretical tools and concepts to be used are the ones of quantum transport through mesoscopic systems, including analytical and numerical methods. In addition, concepts of AI will be studied, developed and applied. The student will work in the <u>Mesoscopic</u> <u>Quantum Physics Team</u> at IPCMS.

[1] M.A. Topinka et al., <u>Science 289</u>, 2323 (2000); <u>Nature 410</u>, 183 (2001)

- [2] H. Sellier et al., <u>Semicond. Sci. Technol. 26, 064008 (2011)</u>; and references therein
- [3] R.A. Jalabert, W. Szewc, S. Tomsovic, and D. Weinmann, *Phys. Rev. Lett.* **105**, 166802 (2010)
- [4] C. Gorini, R. A. Jalabert, W. Szewc, S. Tomsovic, D. Weinmann, Phys. Rev. B 88, 035406 (2013)
- [5] R. Steinacher, C. Pöltl, T. Krähenmann, A. Hofmann, C. Reichl, W. Zwerger, W. Wegscheider, R. A. Jalabert, K. Ensslin, D. Weinmann, T. Ihn, <u>*Phys. Rev. B* 98</u>, 075426 (2018)