Master project: Classical chaos and electron transport in two-dimensional crystals

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The statistical physics you will have studied in your courses has all dealt with systems in equilibrium, where we have powerful formalisms. However, many interesting things happen out of equilibrium, when mass, energy, momentum, are transported. We have no powerful general theory to deal with those kinds of systems. To truly understand what is happening, we must go back to one of the fundamental assumptions of statistical physics: that the systems in question are chaotic.

In this project, you will investigate the connection between chaos and transport in a specific system: classical electrons diffusing in two-dimensional crystals. We know that if the total energy is above a certain threshold, the Knauf threshold, there is always diffusion and chaos in this system. But what happens around this threshold is not clear. Is diffusion possible below the Knauf threshold? If it is, could it be anomalous? How do the diffusion and chaos relate to eachother in the vicinity of the Knauf threshold and how do they depend on the total energy? To answer these questions, you will write your own molecular-dynamics simulation of this system and calculate the diffusion coefficient as well as characterise the chaos.

This project will involve a collaboration with Rainer Klages, School of Mathematical Sciences, Queen Mary University of London. We will discuss with Rainer via skype, and, if possible, also meet in person.

If you are interested in this project, or something like it, don't hesitate to send me an email or drop by my office.

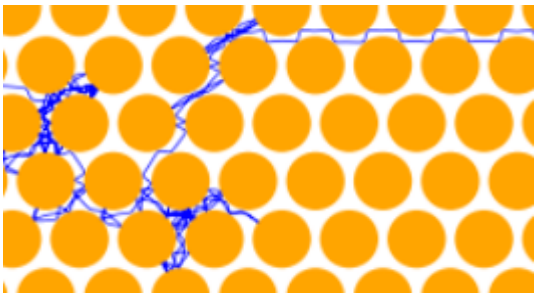

Figure 1: A section of a simulated trajectory of a classical electron in a crystal lattice. The part at the top right, where the trajectory repeats the same motion several times, is a sign that there may be anomalous diffusion.