Doping Mott Insulators:
Band Electrons, Spin Polarons or Fractional Excitations?

Motivation:

All materials around us can be classified by their electrical conductivity. These which easily conduct are called metals (e.g. copper), the ones that have very high resistance are insulators (e.g. diamond) and the ones that can conduct electricity under certain conditions, such as heating, are called semiconductors (e.g. silicon). Interestingly, in *most* of the cases we are able to correctly predict which material belongs to which of these three classes. This is one of the biggest triumphs of the 20th century physics. Interestingly, this classification can largely be understood using the knowledge gained during high school chemistry lessons – since to a large extent it all stems from the understanding of how electrons in atoms forming crystals occupy its shells, as dictated by the so-called Aufbau principle.

This project, however, is about understanding the physics of such 'special' materials whose electrical conductivity can*not* be understood in the above-mentioned manner. The reason for this is that in some crystals, called correlated materials, interaction between the electrons, that decide about their conductive properties, cannot be neglected. This happens for instance in various transition metal compounds (e.g. a copper oxide La_2CuO_4). The problem is that taking such an interaction into account for a real material that consists of an Avogadro number electrons is a tremendously difficult task, due to the exponential growth of the problem complexity with the number of electrons. On the other hand, such studies are highly needed not only out of pure curiosity but also from the utilitarian perspective – for often these correlated materials hold some spectacular properties. Probably the two best examples here are: superconductivity at relatively high temperature found almost 40 years ago in doped copper oxides but whose origin is still unclear *or* the recently discovered extremely tunable (and intertwined) magnetic and electronic properties found in the moiré superlattices of the twisted transition metal dichalcogenides.

Project Goal:

In a general sense, this project is about a class of correlated material problems that might be regarded as being to some extent understood. Yet, as discussed below this can largely be questioned and, besides, several extensions of this understanding are highly needed.

More specifically, we want to consider here what happens when additional electrons are removed and holes are created (so-called 'doping' procedure, well-known in the semiconductor industry) in the Mott insulators. The latter materials constitute some of the simplest examples of correlated matter, for in that case electrons, whose number is commensurate with the number of lattice sites, repel between each other so much that they do not move between atoms and thus the electronic conductivity of the material vanishes. Notably, doping such materials should allow for some electronic motion being possible – just as the traffic jam that comes to a standstill on a motorway lessens once some of the cars leave it. The main goal of the project is to challenge and extend an existing paradigm that tells us how such doped holes move in the Mott insulator *depending* on its magnetic structure.

Description of Research and Substantial Results Expected:

Although the project builds on the previously gained theoretical and experimental knowledge, new analytical and numerical approaches will be developed. For instance, we will apply the recently proposed (and published) method of tackling a one-dimensional doped Mott insulating problem using a very specific language (so-called 'slave-fermion' quantum basis) to a far broader class of problems. As the language used in this method is very intuitive, it should give us the much-needed insight and provide us with clear answers on the issues as well as on the extensions of the above-mentioned paradigm. On the practical side, we expect that some of the key properties of the novel doped Mott insulating materials, in particular their fragility to doping that is exemplified by the sudden changes in electric or magnetic properties, will be way better understood or even theoretically *predicted*. The latter is of ultimate importance for fabrication of novel materials with desired properties.