# Summary

The characterization of a material as metallic or insulating, the study of transitions between such states and the development of suitable models is clearly of great fundamental and practical interest. The one-band Hubbard model is a conceptionally relatively simple model which is potentially relevant in this context since its primary parameter, the on-site interaction $U$ triggers a transition or a crossover from metallic behavior at small $U$ to insulating behavior at large $U$ and half filling. A reduction of complexity of this model is achieved by the dynamical mean-field theory (DMFT); due to its nonperturbative character, this method is reliable in the range of interest, i.e., for intermediate to strong coupling. The resulting model certainly misses important properties of specific materials such as $V_2O_3$; nevertheless, it is a good candidate for controlled numerical studies of the more abstract metal-insulator transition (MIT) problem.

We have presented quantum Monte Carlo (QMC) results for a fully frustrated version of the Hubbard model and constructed its phase diagram. We have resolved a controversy regarding the existence and extent of the MIT coexistence region and have succeeded in the precise determination of the first-order transition line; a task that was previously considered too difficult for numerically exact methods. The new methods employed for this purpose and a more direct (and yet untested) approach developed in this work should prove fruitful for broader application in the future. Further research will also profit from our discovery and correction of problems in some implementations of the QMC method.

The MIT phase diagram Fig. 3.50, a main result of this work, clearly does not represent a complete scenario for any material featuring a MIT. This follows already from the finite (and large) entropy predicted in the insulating ground state which violates Nernst's law. This contradiction may to some degree be regarded as an artifact of the DMFT limit: For any fixed disorder distribution and finite hopping range, long-range order is expected to set in below some critical temperature in any finite dimension $d$. A more realistic and consistent DMFT description is possible when the low-temperature phase is ordered already in $d = \infty$, i.e., for partial frustration. We have discussed the qualitative implications of variable frustration in the (nongeneric) case that the properties of the paramagnetic phase remain unchanged. The question whether the topology of the phase diagram of $V_2O_3$ (with a first-order paramagnetic metal-insulator transition and an antiferromagnetic low-temperature phase) can be reproduced for a lattice with realistic frustration is still open.

The theory of transport in infinite dimensions was previously restricted to the hypercubic lattice (or anisotropic stacked lattices) with nearest-neighbor hopping.