Density functional theory and dynamical mean-field theory: A way to model strongly correlated systems

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by

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Chapter 1

Introduction

1.1 Introduction into correlated electron materials

The concept of electronic correlations is one of the hardest, yet most interesting aspects in the field of theoretical as well as experimental solid state physics. This thesis will investigate the realisations of strong electronic correlations due the Coulomb repulsion between electrons in different materials and theoretical concepts of describing and investigating their effects on physical properties.

In this chapter we will give a short overview over the main aspects of this thesis. We will first introduce the very general problem of how an ensemble of electrons in a solid interacts and what problems arise when we want to investigate the system from the viewpoint of a theoretical physicist.

After that, we will review a special type of materials, namely a class of superconductors in which electronic correlations are important to consider for a correct physical description and interpretation of their properties.

Chapter 2

Methods

2.1 The Hubbard model

In order to find a way of appropriately treating electronic correlations we should also consider alternative ways of treating the Coulomb repulsion. Since the Coulomb interaction is a long-range interaction due to the potential falling off as $\sim \frac{1}{r}$, the problem is notoriously difficult since we need to take the contribution of many particles into account. However, in real systems the range of the interaction is effectively reduced due to screening effects of the electronic charge. Consider electrons moving in a positive background potential given by the atomic lattice. Focussing on a specific electron, one will observe a region of reduced electronic density in the vicinity of said electron due to the Coulomb repulsion, that creates an effective positively charged cloud that will move around with the electron. From large distances, the resulting potential seen by other electrons will thus be reduced by the positive cloud compared to the bare electron. Therefore, the effective potential will fall off much faster than the bare Coulomb repulsion, making it an effective short-range interaction. This is why approximative models like the Hubbard model [1, 2, 3], which assume the Coulomb repulsion to be completely local, can be quite appropriate to describe correlated lattice systems.

The most simple variant is the one-band fermionic Hubbard model, given by the Hamiltonian

$$H = \sum_{\langle i,j\rangle,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{2.1.1}$$

with the hopping amplitudes t_{ij} between neighbouring sites i, j. The Coulomb interaction is represented by a local on-site interaction U, that has to be paid if two electrons of opposite spin occupy the same site. Fig. 2.1 shows an example of the two-dimensional Hubbard model. It can encompass basically all types of lattice systems by appropriately choosing the hopping integrals t_{ij}. Even though this model appears to be very simple, it is not only impossible to be solved analytically in more than one dimensions [4], but also includes

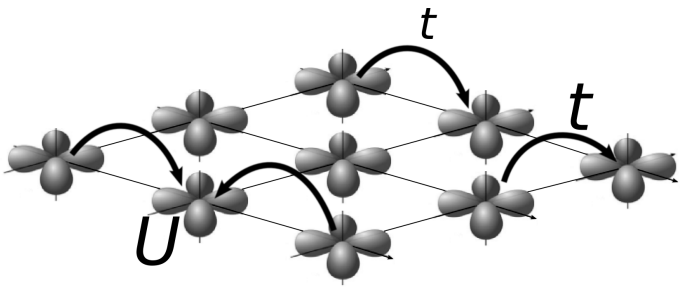

Figure 2.1: Illustration of the one-band Hubbard model in two dimensions. The model consists of a lattice of atomic sites occupied by electrons that can hop between neighbouring sites with the hopping amplitude t. Double occupation of an atomic site with two electrons of the opposite spin incurs an energy penalty of U to mimic the screened short-range Coulomb interaction. .

the main effects of the competition between the kinetic energy and Coulomb interaction. Considering for example the limit $U/t \to 0$, the Hamiltonian corresponds to that of free particles with a dispersion corresponding to the Fourier transform of t_{ij} For the linear chain we already had as an example $\epsilon(k) = -2t\cos(ka)$ and, since the Hamiltonian separates into a sum of single-particle terms, all expectation values can be calculated independently. Thus, all correlation functions factorize, e.g.

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle. \tag{2.1.2}$$

Considering the other limit of $U/t \to \infty$, the Hamiltonian becomes just the sum of the double occupations times U. At half filling the ground state which minimizes the energy thus corresponds to each electron being localized on an atomic site with zero probability on all other sites. As a result, the system is now in an insulating state due to the electronic correlations and the correlation functions no longer factorize

$$\underbrace{\langle n_{i\uparrow} n_{i\downarrow} \rangle}_{=0} \neq \underbrace{\langle n_{i\uparrow} \rangle}_{=0.5} \underbrace{\langle n_{i\downarrow} \rangle}_{=0.5}. \tag{2.1.3}$$

Thus, even though the Hubbard model is quite simple, it can show the non-trivial effect of a as U/t is increased. Approximations like Hartree-Fock theories that are based on the separation of correlation functions are, therefore, also insufficient to correctly describe the physics in the Hubbard model for strong interactions.

Chapter 3

Result & Interpretation

3.1 First experiment

3.2 Second experiment

Chapter 4

Conclusion & Outlook

References

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