Magnetism in transition metals and their oxides

K. Held M. Ulmke D. Vollhardt

Theoretische Physik III, Elektronische Korrelationen und Magnetismus
Universität Augsburg, 86135 Augsburg, Germany

Email: Held@Phyik.Uni-Augsburg.DE

LRZ-Account: b5101bh, b5101bu

Abstract

Metallic ferromagnetism is in general a problem arising in systems with strong Coulomb interaction. Since there do not exist systematic analytic methods to investigate such types of problems, the microscopic origin of metallic ferromagnetism is still not sufficiently understood. Here, we employ quantum Monte Carlo simulations within dynamical mean-field theory to solve simplified models for transition metals and manganites with the aim to gain insight into the microscopic conditions favoring ferromagnetism.

Keywords: Quantum Monte Carlo simulations; correlated electron-systems; ferromagnetism

1 Introduction

What is the microscopic origin of ferromagnetism? Seventy years ago, in 1928, Heisenberg addressed this question [1] after having discovered the phenomenon of quantum mechanical exchange and the corresponding exchange interaction. He formulated a spin model (the Heisenberg model), hoping to be able to answer precisely this question. However, it was pointed out by Bloch [2] that a model of localized spins cannot explain *metallic* ferromagnetism as observed in iron, cobalt and nickel, and that a proper model would have to include the itinerancy of the electrons, i.e., the kinetic energy. Based on the observation that the Curie temperature is of order 10^3 Kelvin (0.1 eV) in these systems it is clear that the kinetic and the electrostatic energies, i.e. the spin-*in*dependent Coulomb interaction, together with the Pauli principle must ultimately be responsible for metallic ferromagnetism. Ever since one has been looking for the simplest microscopic model and mechanism explaining the origin of metallic ferromagnetism. Today we know that even with the "rightmodel the answers are not easily obtained since metallic ferromagnetism generally occurs only at strong Coulomb interactions and off half filling of the bands [3, 4]. Thus, it belongs to the class of problems for which systematic theoretical approaches do not exist. Namely, weak-coupling theories or renormalization group approaches which are so effective in detecting instabilities with respect to antiferromagnetism or superconductivity, do not work in this case. Instead, *non-perturbative* methods are required, such as the *numerical simulation* of these models, e.g., by means of quantum Monte Carlo simulations.

2 Method: Quantum Monte Carlo simulation

Without the Coulomb interaction, which is so crucial for ferromagnetism, the solution of the microscopic models considered would be an easy problem. In this case, every electron is independent of the others and only the eigenvalues of a simple one-electron Hamiltonian need to be calculated to describe the entire system. The idea of the *quantum* Monte Carlo (QMC) method is to replace the system of electrons with Coulomb interaction by a system of non-interacting electrons. This is possible by means of a Hubbard-Stratonovich transformation. However, the prize for this simplification is that one obtains a high-dimensional sum or integral over different

non-interacting systems. While every summand corresponds to a simple matrix problem, the large number of summands makes an exact summation impossible. Here, the Monte Carlo method enters which makes the calculation of the high-dimensional sum feasible (up to a statistical error).
The effort of the finite-cluster QMC algorithm (number of floating point operations) is

$$\text{FLOP} = kT^{-2}N^3M^2 \tag{1}$$

where T is the temperature, N the number of lattice sites (transition metal ions) considered, and M the number of orbitals per site taken into account. Note, that the prefactor k is very large ($10^3 - 10^6$ if T is given in eV) due to the Monte Carlo summation. For just one orbital ($M = 1$) and room temperature simulations of up to about 10^3 sites are possible but only for special physical parameters where the QMC simulation does not suffer from the so called "sign-problem" (here, the statistical error grows exponentially with T, N, and M). In particular in many cases of physical interest, the "sign-problem" makes a direct simulation of a finite-size cluster impossible. Furthermore, even without sign-problem a system of $N = 10^3$ sites is still far away from the thermodynamic limit ($N \to \infty$) which is the proper description of a solid-state system which has a size of typically 10^{23} sites.
To overcome these difficulties, we employ the dynamical mean-field theory (DMFT) [5] which becomes exact if the number of neighboring sites (Z) goes to infinity ($Z = 6$ for a simple cubic lattice; $Z = 12$ for a face-centered cubic lattice). The DMFT allows a direct evaluation in the thermodynamic limit and is an approximation controlled in the small parameter $1/\sqrt{Z}$. It was successfully applied and found to be a reliable approximation without "sign-problem". Even within DMFT, an analytic evaluation is not possible without further approximations, but the numerical solution by QMC simulations with the Hirsch and Fye [6] algorithm is manageable. The numerical effort within DMFT grows like

$$\text{FLOP} = kT^{-3}M^2, \tag{2}$$

typical matrix sizes for the non-interacting problem are 100×100 to 500×500, and the algorithm vectorizes well. More information concerning vectorization and parallelization can be found in the contribution by Blümer et al..

3 Results I: One-band Hubbard model on frustrated lattices

The simplest microscopic model containing the basic ingredients for ferromagnetism, i.e., the itinerancy of the electrons and the Coulomb interaction, is the one-band Hubbard model which was proposed independently by Gutzwiller, Hubbard, and Kanamori in 1963, with the explanation of metallic ferromagnetism in 3d transition metals in mind. However, it was found in the following years that this model is rather generic for antiferromagnetism. Only recently, it become clear that it does describe ferromagnetism if lattices are considered on which antiferromagnetism is frustrated like the face-centered cubic lattice. This progress in our understanding of the Hubbard model is to a large extent due to the numerical investigations in dimension $d = 1$ [7], $d = 2$ [8], and within the DMFT ($d = \infty$) [9].

4 Results II: Orbital degeneracy and Hund's rule coupling

The Hubbard model only takes into account one orbital per site while the 3d orbitals of the metallic ferromagnets iron, cobalt, and nickel are five-fold degenerate. This band degeneracy leads to additional intra-atomic Coulomb interactions, in particular, the intra-atomic (ferromagnetic) exchange interaction between electrons in different orbitals. These "Hund's rule couplings" are the origin of Hund's first rule which says that the spins on an isolated atom are aligned ferromagnetically. Slater [10] and van Vleck [11] suggested that this "atomic magnetism" may be transmitted from one atom to another by the itinerancy of the electrons.
Recently, this mechanism has attracted wide attention [12]. However, except for some very special fillings (for one such filling the degenerate model was known to have an *insulating* ferromagnetic ground state for a long time [13]) the degenerate model is difficult to treat. Here, new insight was gained by QMC calculations within DMFT which show that Hund's rule coupling is an effective mechanism that stabilizes also *metallic* ferromagnetism in a broad range of fillings [14].
Different quantities, like the spectral function, the phase diagram, and the dependence of the ferromagnetic

transition temperature on volume, where investigated to find characteristic features for the two basic mechanisms for ferromagnetism: frustrated lattices and Hund's rule coupling. However, it was found that despite the different underlying origin the physics described by both mechanisms is similar.

5 Results III: Models for manganites

Currently, "colossal magnetoresistance" (CMR) manganites attract most intensive interest because of the drastic change of the resistivity in an external magnetic field, i.e., the CMR effect [15]. The origin of the CMR is a transition from an "insulating" paramagnetic to a metallic ferromagnetic phase. For manganites, the so-called double exchange mechanism [16] which can be described microscopically by the ferromagnetic Kondo lattice model is generally considered to be the origin of ferromagnetism. However, it was pointed out by Millis et al. [17] that double exchange alone cannot describe the resistivity of manganites, and the effect of the coupling between electronic and lattice degrees of freedom was stressed. Another important aspect missing in the Kondo lattice model is the Coulomb interaction. Up to now, the latter was only considered in special limits due to technical difficulties of the ensuing many-body problem. Since this problem is tractable within DMFT we employed this approach [18] and found that the Coulomb interaction is certainly important for understanding CMR manganites and that double exchange gives only an appropriate description for a certain range of filling. Instead, another mechanism, i.e., superexchange, becomes effective. The crossover from double exchange to superexchange yields a maximum in the paramagnetic-ferromagnetic transition temperature in qualitative agreement with experiment.
Despite some progress, the unusual properties of the "insulating" paramagnetic phase remain an open question for the future.

Publications [9, 14, 18, 19] which arose from this project can be down-loaded via
http://www.physik.uni-augsburg.de/theo3/publications.de.shtml.

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