Magnetic phases of the two orbital Hubbard model in dynamical mean field theory

R Peters¹, T Pruschke¹
¹ University of Goettingen, 37077 Goettingen, Germany
E-mail: peters@theorie.physik.uni-goettingen.de

Abstract. We examine the two orbital Hubbard model within dynamical mean field theory. The two orbital Hubbard model is the basic model for treating strongly correlated electrons in degenerate \( e_g \)-bands, as found for example in the manganites. We have calculated the magnetic phases of the model for different interaction values and fillings of the system at \( T = 0 \).

1. Introduction
The physics of magnetic materials typically involves partially filled d- or f-shells [1, 2]. On the one hand, these states are usually rather localised, which is the origin of strong electron-electron interactions. On the other hand, the orbital degeneracy of the d- or f-states leads to the coupling of spin, charge and orbital degrees of freedom, which in fact is one ingredient leading to magnetism. It is thus not astonishing that these materials show a very rich ground state phase diagram with a variety of different ordered phases [2]. A very interesting example are the well known manganites [3, 4]. Here the 3d-shell splits due to cubic lattice symmetry into a partially filled \( e_g \) and a completely filled \( t_{2g} \) band, the latter being frequently treated as localised spin \( S = \frac{3}{2} \).

In this article we focus on the situation of strongly correlated electrons in an \( e_g \)-band. The basic model for this situation is the two orbital Hubbard model [5, 6, 7, 8]

\[
H = \sum_{ij,\sigma} \sum_{m=1}^{2} t_{ij} c_{i,\sigma,m}^{\dagger} c_{j,\sigma,m} - \mu \sum_{i,\sigma} \sum_{m=1}^{2} n_{i,\sigma,m} \\
+ U \sum_{i} \sum_{m=1}^{2} n_{i,\uparrow,m} n_{i,\downarrow,m} + (U' - J/2) \sum_{i} (n_{i,\uparrow,1} + n_{i,\downarrow,1})(n_{i,\uparrow,2} + n_{i,\downarrow,2}) \\
- 2J \sum_{i} \vec{S}_{i,1} \cdot \vec{S}_{i,2}.
\]

Here \( i, j \) are indices of lattice sites; \( m \) is the orbital index, which can be 1, 2 and \( \sigma \) is the spin index. So \( c_{i,\sigma,m}^{\dagger} \) creates an electron at site \( i \) in orbital \( m \) with spin \( \sigma \). \( \mu \) represents the chemical potential with \( n = c^{\dagger} c \) being the density operator. The two particle interaction is taken as in [8], but we neglect the two particle hopping term \( J c_{i,\sigma,m}^{\dagger} c_{i,\sigma,n}^{\dagger} c_{i,\sigma,n} c_{i,\sigma,m} \) [9]. This is done mostly because of numerical reasons and must be considered as approximation. Therefore, in our model the two particle interaction can be understood as a local intra band interaction with
amplitude $U$, a local inter band interaction with amplitude $U' - J/2$ and a Hund’s coupling with amplitude $2J$ between the spins $\vec{S}_1$ and $\vec{S}_2$ of the two orbitals. The natural energy scale of the non interacting system is the bandwidth $W = 4t$. We also neglect the $t_{2g}$ spin for the time being. It’s influence will be discussed in a forthcoming publication.

The equivalence between the orbitals would impose $U' = U - 2J$ [8]. But in this article we want to treat all three parameters $U$, $U'$ and $J$ as independent, which can be the situation in real materials due to further reduced local symmetry. For calculating the ground state phase diagram we use the dynamical mean field theory (DMFT) [10, 11]. By relating the lattice problem to a self-consistent quantum impurity model, the DMFT completely includes the local quantum mechanics of the problem. For solving the quantum impurity model, we used the Numerical Renormalisation Group (NRG) [12, 13]. We performed our calculations with a semi elliptic density of states, which corresponds to a Bethe lattice in infinite dimensions.

2. Results

2.1. Anti- and Ferromagnetism for $1 < n < 2$

We performed calculations for local interactions $U \geq 2W$, as we were interested in the physical situation present in transition metal oxides, which usual show a large value for the local interaction strength [2]. The magnetic phase diagram of the one orbital Hubbard model for such interactions strengths only shows an antiferromagnetic phase exactly at half filling [14, 15]. This phase cannot be doped, but there is a phase transition to an incommensurate phase near half filling which eventually gets unstable towards a paramagnetic phase. The phrase incommensurate is here used for a non-convergent DMFT calculation, in which the polarisation oscillates. Unfortunately, we cannot stabilise these states, but there is evidence by other authors [16] that the stable state in these parameter region is an incommensurate spin density phase. We will use the phrase incommensurate in this context throughout this article.

It is therefore not surprising to find that the antiferromagnetic phase at half filling cannot be doped in the two orbital case with large local interaction, too, and that we also find such an incommensurate magnetic order around half filling. Figure 1 shows a schematic phase diagram for an average occupation $\langle n \rangle = 1.5$ of the system. The points in the figure denote the parameters where we performed calculations. The two orbital model is an extreme case for the application of the NRG. The reliable calculation of a spectral functions needs in this case approximately 15Gb of shared memory and several CPU hours for completing the NRG. As we typically need of the order of 20 - 50 DMFT iterations for converged solutions with magnetic order, the small amount of points in the diagram is explained. Nevertheless, the ones calculated give us a clear picture of the physics.

The phase diagram shows large regions with magnetically ordered phases [17, 18, 19, 20, 21, 22, 23]. Only for small values of both $U'$ and $J$ the system prefers the paramagnet. The magnetic instability is clear due to the fact, that a large $U$, in this case $U/W = 4$, results in strongly localised states. For not too large values of Hund’s coupling $J \approx W/2$ the antiferromagnetic superexchange coupling usually dominant close to half filling is strong enough to create an incommensurate spin structure even here. For increasing Hund’s coupling the system forms a ferromagnetic ground state [17, 22] due to double exchange now winning over superexchange type correlations. If one looks again at the Hamiltonian, one sees that for $J > 2U'$ the effective inter orbital density-density interaction changes from repulsive to attractive. In this parameter region it is very difficult to stabilise a doped system. The attractive interaction pulls the system to half filling or an empty system. There are only a few parameter points where we could stabilise a solution for $n = 1.5$. There the ground state of the system seemed to be an incommensurate phase again. The physical relevance of this parameter regime with $J \approx U'$ is disputable on purely electronic grounds, as such large Hund’s coupling are rather unusual. However, inclusion of Jahn-Teller phonons may in fact induce negative $U'$, and consequently charge instabilities.
Figure 1. Schematic ground state phase diagram for $\langle n \rangle = 1.5$ for different values of $U'$ and Hund's coupling $J$ and $U = 4W$ fixed. IC stands for a magnetic phase with an incommensurate spin structure. Points denote the parameters where the calculations were performed. Lines are meant as guide to eye.

We also performed calculations for $U = 3W$ and $U = 2W$. The size of the ferromagnetic phase shrinks with decreasing local interaction and the paramagnetic region gets more and more pronounced. For the $U = 2W$ we found no ferromagnetic state for occupations $1.1 < n < 1.5$ for $U', J < U$.

2.2. Quarter filling
For a bipartite lattice quarter filling again represents a special situation where one can expect new ordered phases in our model. Figure 2 shows the ferromagnetic phase exactly at quarter filling for $U = 4W$. Here we found two different ferromagnetically ordered ground states. For large enough Hund’s coupling the ferromagnetic state observed already at $n = 1.5$ extends to occupations smaller than one. For large enough repulsive inter orbital density-density coupling, on the other hand, there exists an orbitally ordered ferromagnetic phase [18, 21, 20, 23], which can only be found exactly at quarter filling. There seems to be a direct first order transition between both ferromagnetic states.

3. Conclusions
We analysed the magnetic ground state phase diagram of the two orbital Hubbard model within the DMFT. For stabilising magnetic order away from half filling a large on site interaction is needed. For values $U = 4W$ we found extended regions of incommensurate spin chiral waves and ferromagnetic regions for $1 < n < 2$. Exactly at quarter filling $n = 1$, we found an additional orbitally ordered ferromagnet for large $U'$, and one can observe a phase transition between a homogeneous and an orbital ordered ferromagnet.
Figure 2. Ferromagnetic phase at quarter filling for $U = 0.8$, $W = 0.2$ for different $J$ and $U'$. The red points denote an orbitally ordered ferromagnet, while the violet points denote a homogeneous ferromagnet. For very small Hund’s coupling the system is in a paramagnetic or incommensurate phase. The line is meant as guide to the eye.

Acknowledgments
We acknowledge financial support by DFG through PR298/10. Computer calculations were done at Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen (GWDG) and at Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen (HLRN).

References
[1] Stöhr J and Siegmann H 2007 Magnetism: From Fundamentals to Nanoscale Dynamics Springer, Berlin
[2] Imada M, Fujimori A and Tokura Y 1998 Rev. Mod. Phys. 70 1039
[3] Coey J, Viret M and Molnar S 1999 Advances in Physics 48 167
[4] Salamon M and Jaime M 2001 Rev. Mod. Phys. 73 583
[5] Hubbard J 1963 Proc. R. Soc. A 276 238
[6] Kanamori J 1963 Prog. Theor. Phys. 30 275
[7] Gutzwiller M 1963 Phys. Rev. Lett. 10 159
[8] Oleš A 1983 Phys. Rev. B 28 327
[9] Pruschke T and Bulla R 2005 Eur. Phys. J. B 44 217
[10] Georges A, Kotliar G, Krauth W and Rozenberg M 1996 Rev. Mod. Phys. 68 13
[11] Pruschke T, Jarrell M and Freericks J 1995 Adv. in Phys. 44 187
[12] Wilson K 1975 Rev. Mod. Phys. 47 773
[13] Bulla R, Costi T and Pruschke T 2008 Rev. Mod. Phys. 80 395
[14] Zitzler R, Pruschke T and Bulla R 2002 Eur. Phys. J. B 27 473
[15] Peters R and Pruschke T 2009 New J. Phys. 11 083022
[16] Freericks J and Jarrell M 1995 Phys. Rev. Lett. 74 186
[17] Fresard R and Kotliar G 1997 Phys. Rev. B 56 12909
[18] Held K and Vollhardt D 1998 Eur. Phys. J. B 5 473
[19] Momoi T and Kubo K 1998 Phys. Rev. B 58 R567
[20] Fresard R, Raczkowski M and Oleš A 2005 Phys. Stat. Sol. B 242 370
[21] Oleš A 2003 Phys. Stat. Sol. B 236 281
[22] Sakai S, Arita R and Aoki H 2007 Phys. Rev. Lett. 99 216402
[23] Kubo K 2009 Phys. Rev. B 79 020407