Orbital and magnetic order in the two-orbital Hubbard model

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We examine the orbital and magnetic order of the two-orbital Hubbard model within dynamical mean-field theory. The model describes the low-energy physics of a partially filled e_g band as can be found in some transition metal compounds. The model shows antiferromagnetic as well as ferromagnetic phases. For stabilizing ferromagnetism we find that Hund's coupling is particularly important. Quarter filling represents a very special situation in the phase diagram, where the coupling of spin, charge, and orbital degrees of freedom are involved. Exactly at quarter filling we find a metal insulator transition (MIT) between two almost fully polarized ferromagnetic states. This MIT can be tuned by changing the local interaction strength and seems to be a first order transition at zero temperature. Apart from these ferromagnetic states we were also able to stabilize antiferromagnetic and charge ordered phases at quarter filling, depending on the interaction parameters.

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I. INTRODUCTION

Magnetism is still a very important topic in condensed matter physics. Analyzing the elements involved in magnetic materials, one has to conclude that the existence of magnetism is intimately connected to the presence of partially filled d or f shells. It is thus not surprising that understanding the influence of these shells on the low-temperature physics is crucial for a proper description of magnetic materials.

Since d or f shells are typically more strongly localized than the s or p shells of simple metals or semiconductors, they often are subject to strong correlation effects making their theoretical study a challenging task. In this context very interesting materials are the transition metal oxides.[1,2] One prevalent lattice structure of transition metal oxides is the cubic perovskite, in which the transition metal atom sits in the center of an oxygen octahedron. The states relevant at low temperatures are the d orbitals of the transition metal atom. Due to the cubic crystal symmetry the d orbitals split into a threefold degenerate t_{2g} and a twofold degenerate e_g band, which for the coordination present in the perovskite structure has the higher energy compared to the t_{2g} band. Thus not only strong correlations but also orbital degeneracy plays an important role in the physics of these compounds.

To give a specific example for a transition metal oxide, let us consider the manganites,[3–8] or more precisely $La_{1-x}Ca_xMnO_3$. Manganites became famous for their colossal magneto resistance. Besides this particular feature they show a very rich phase diagram with different magnetic and orbitally ordered phases. In $La_{1-x}Ca_xMnO_3$ one has to distribute $4-x$ electrons per site to the d states of the manganese according to Hund's rules. Thus, the electronic configuration in this compound can be modeled by a partially filled e_g band close to quarter filling and a half filled t_{2g} band which couples via Hund's coupling ferromagnetically to the e_g electrons. The hopping between the t_{2g} states is very small and thus the t_{2g}-states are often modeled as localized $S=3/2$ spins. Besides this electronic part the lattice degrees of freedom and especially Jahn-Teller distortions are important to correctly describe the physics of manganites.[9]

The ultimate goal surely is to theoretically describe the properties of materials like $La_{1-x}Ca_xMnO_3$ including all the degrees of freedom mentioned before. However, at least equally important for a proper microscopic understanding of the physics is to disentangle the contributions of the different degrees of freedom and identify the individual influence, in particular to what extent a certain degree of freedom is responsible for effects or just follows the lead.[10] For this reason we now leave the special topic of manganites and focus on the role of the electronic degrees of freedom, in particular the role of interactions on the magnetic and orbital properties of a degenerate e_g band. We thus ignore effects of the t_{2g} spin and the lattice in the following. Based on such an investigation, one can later include further features such as different band widths of the e_g band,[11–15] or additional degrees of freedom, for example the t_{2g} spin (or band), respectively, the strong coupling to the lattice, step by step, thereby properly identifying for which particular features they are actually responsible. As we will discuss, already the simplified situation with only an e_g band present shows very complex ground-state properties, involving the coupling of charge, spin, and orbital degrees of freedom.

The article is organized as follows: after this introduction we establish the model and discuss the methods we have used for solving it. In the results section we first analyze the situation for a band filling between quarter filling and half filling. In the second part of the results section we particularly address quarter filling representing a very special point in the phase diagram, at which different ordered phases compete with each other.

II. MODEL AND METHOD

We model the e_g band as a two-orbital Hubbard model[16–20]

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

Here i,j label the lattice sites; $m=1,2$ is the orbital and σ the spin index. Thus, $c^{\dagger}_{i,\sigma,m}$ creates an electron at site i in orbital m with spin σ. As usual, μ represents the chemical potential with $n=c^{\dagger}c$ being the density operator. Note that, in the spirit of the philosophy discussed in the introduction, we assume the same band structure and width for both orbitals in the e_g band and also do not include orbitally off diagonal hopping.

The two particle interaction is parametrized as in Ref. 20, but we neglect the two particle hopping term $Jc^{\dagger}_{i,\uparrow,m}c^{\dagger}_{i,\downarrow,m}c_{i,\downarrow,n}c_{i,\uparrow,n}$.[21] This is done mainly for numerical reasons, as otherwise one cannot introduce a conserved orbital quantum number. This of course introduces an additional approximation; however, previous studies indicated that this particular term is of minor importance, at least for ferromagnetic Hund's exchange, while the inclusion of the rotationally invariant spin exchange appears to be crucial.[21] Therefore, in our model the two particle interaction is given as a local intraband interaction with amplitude U, a local interband 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.

In order to investigate the possible magnetically, orbitally, and charge ordered phases of the two-orbital model we use the dynamical mean-field theory (DMFT).[22,23] As this mean-field theory properly includes the local dynamics due to electronic correlations, it accounts for such subtle effects such as crossover between itinerant and localized order[24] and strong reduction of transition temperatures. As it is well-known, the lattice structure enters the DMFT calculation only via the noninteracting density of states (DOS). Since we are interested in general qualitative aspects of ordering phenomena in the two band model and not in the description of a particular material, we can use this property and choose a numerically convenient form of the DOS. As has been discussed extensively,[22] the semielliptic DOS obtained from a Bethe lattice with infinite coordination number is indeed a numerically convenient choice, which also allows to address the ordered structures we are interested in, namely antiferromagnetic Néel, homogeneous ferromagnetic, as well as charge and orbital order. More complex structures such as for example ferromagnetic order in one direction and antiferromagnetic in another[25] are excluded deliberately.

The DMFT self-consistency maps the lattice onto an effective impurity Anderson model, which in the present case becomes a two-orbital Anderson model. We solve this Anderson model with the numerical renormalization group (NRG),[26,27] which allows us to calculate properties for wide parameter regions at $T=0$. To reliably calculate spectral function with NRG we use the complete Fock space method.[28,29] It must be noted that the two-orbital model is an extreme case for calculating spectral functions within the NRG. The calculation of one spectral function requires approximately 15 GB shared memory and several CPU hours. As discretization parameter within the NRG we used $\Lambda=2$, keeping up to 5000 states per NRG step in a typical calculation.

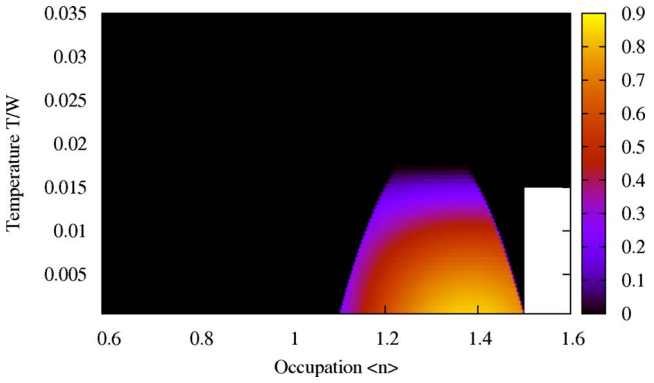

FIG. 1. (Color online) Ferromagnetic polarization for $J=W$ as function of filling at $U=4W$, $U'=U-2J$, and $T=0$. For fillings $n>1.5$ we observe signs of an incommensurate spin-density wave extending to half filling. The phase diagram was created by fitting a smooth surface through approximately 40 inhomogeneously distributed data points. Therefore the location of the phase boundaries are only meant as rough sketches.

III. RESULTS

A. Filling range $1<\langle n\rangle\leq 2$

Let us begin the discussion of our numerical results by an overview of the magnetic phase diagram as function of filling for $1<\langle n\rangle\leq 2$. The calculations were carried out using a fixed local intraorbital interaction $U/W=4$. Here, W is the bandwidth of the semielliptic DOS, which will be used as energy scale throughout this article. This strength of the interaction is a good guess for transition metal oxides. As in the one orbital Hubbard model,[30,31] we also observe that for strong local interaction and half filling the physics is dominated by an antiferromagnetic insulator originating from super exchange.[32] The Néel temperature does not depend on J or U' within the temperature resolution given by the NRG, as long as U is the dominating interaction. The antiferromagnetic phase can be doped resulting in an incommensurate spin density wave away from half filling, which can extend to occupations $\langle n\rangle\approx 1.5$. This is again the behavior expected for strong local interaction.[31] Note that by virtue of the self-consistency only phases commensurate with the lattice structure can be stabilized by a DMFT calculation, but not a truly incommensurate phase. Instead, we rather observe oscillations in the magnetization and occupation during the DMFT self-consistency cycle. Together with evidence from the one orbital model we can conclude that these oscillations, appearing when doping the Néel state at half filling, are indeed signs of an incommensurate spin density wave.[33–35] For occupations of $\langle n\rangle\lesssim 1.5$ the physical situation starts to become influenced by the double exchange mechanism[36,37] and we thus expect to find ferromagnetic order.[38–45] Figure 1 and 2

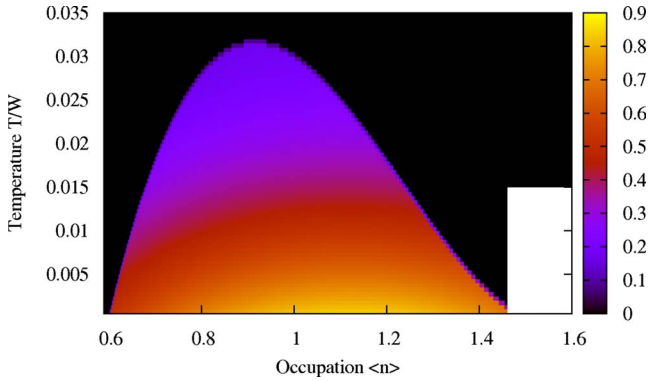

FIG. 2. (Color online) The same as in Fig. 1 for $J=1.5W$. Compared to $J=W$ the ferromagnetic phase extends to higher temperatures and larger hole doping.

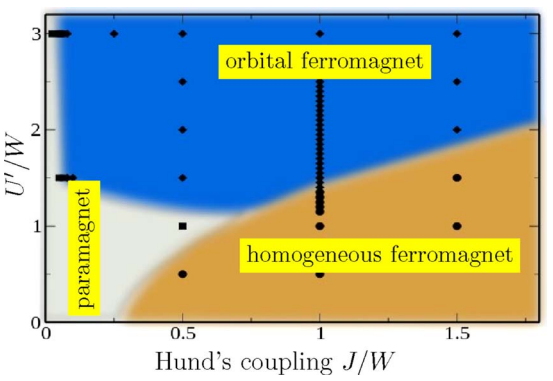

FIG. 3. (Color online) Ferromagnetic order at quarter filling for $T=0$ and $U=4W$ as function of U' and J. Tuning Hund's coupling and the interorbital density-density interaction, one can observe a transition between an orbitally ordered ferromagnetic insulator and orbitally degenerate ferromagnetic metal. The symbols denote the parameters for which calculations were actually performed. The phase boundaries are fits to the calculated points and meant as guide to the eye.

display the ferromagnetic polarization versus the occupation for two values of the Hund's coupling J for fixed $U=4W$ and $U'=U-2J$. One can see how the ferromagnetic phase is stabilized at fillings $n \lesssim 1.5$. The blank rectangles close to half filling in Figs. 1 and 2 represent the already mentioned parameter regimes where we found no convergent solution to the DMFT, but an oscillatory behavior we interpreted as spin-density waves. As they cannot really be stabilized, the true phase boundaries cannot be determined in this parameter region.

As the ferromagnetic double exchange is mostly due to the Hund's coupling, it is not surprising that for increasing Hund's coupling the ferromagnetic state is stabilized up to higher temperatures and larger doping and can even extend beyond quarter filling. However, one must emphasize that Hund's coupling alone is not sufficient to enforce ferromagnetic order in the two-orbital model. We furthermore observe that one in addition needs a rather strong interaction parameter U to stabilize extended regions of ferromagnetism. For example, for $U/W=2$ we found no ferromagnetism for $1 < n < 2$.

B. Magnetic phases at quarter filling, $\langle n \rangle = 1$

Quarter filling such as half filling, represents a very special point for the two-orbital Hubbard model. In a classical picture there is one electron per site, which can choose between two-orbitals. This picture makes already clear that orbital degeneracy and fluctuations will play an important role at quarter filling. In Fig. 3 we show the ferromagnetic ground-state phase diagram for $n=1$ as function of U' and J. As noted before, for strong Hund's coupling J and moderate U' we obtain the orbitally homogeneous ferromagnetic phase discussed in Fig. 2. However, for large enough repulsive interorbital density-density interaction U', we observe that the ferromagnetic spin alignment is accompanied by an antiferroorbital order of the conventional Néel type.[39,45–47] There is a first-order transition between the orbitally ordered ferromagnetic state and the homogeneous one: both the magnetic and orbital polarization show jumps when crossing the phase boundary, see Fig. 4. Note that both states are strongly polarized, i.e., the jump in the magnetization is comparatively small. A more important aspect is that the orbitally ordered ferromagnetic phase is an insulator, while the homogeneous one is a metal. This particular difference becomes apparent from Fig. 5, which shows the spectral function of both ferromagnetic states at quarter filling. The left (right) panel illustrates the spin and orbital configuration of the metallic (insulating) phase in the upper part and the spectral function corresponding to that phase in the lower part. The Fermi energy lies at $\omega=0$. As can be easily seen, the homogeneous ferromagnetic state has a large spectral weight at the Fermi energy, thus representing a metallic system. On the other hand, the orbitally ordered ferromagnetic state has a gap around the Fermi energy, thus representing an insulating state. The gap width of the insulating state decreases when approaching the transition line. Thus, by varying Hund's coupling J or the interorbital interaction U' one can observe a MIT between two almost fully polarized ferromagnetic

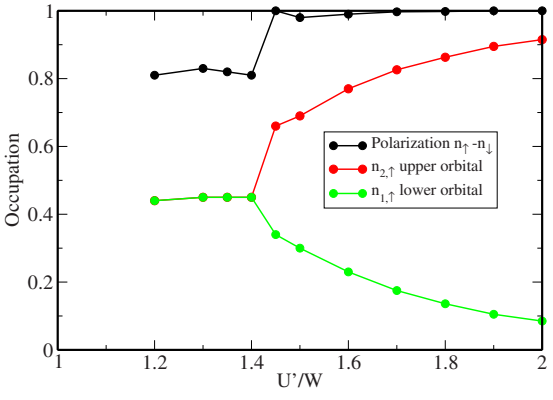

FIG. 4. (Color online) Orbital occupation $\langle n_{m,\uparrow} \rangle$ (m denotes the orbital) and spin polarization for $U/W=4$, $J/W=1$, $T=0$, and different interaction strengths U'. At $U'/W \approx 1.4$ the transition between the homogeneous ferromagnetic state ($U'/W < 1.4$) to the orbital ordered ferromagnet ($U'/W > 1.4$) occurs. Lines are meant as guide to the eye.

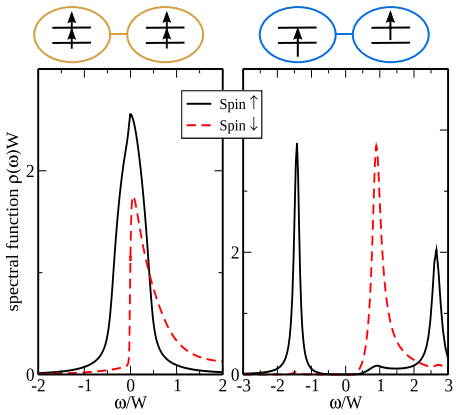

FIG. 5. (Color online) Spectral function and sketch of the electronic configuration. Left panel: metallic ferromagnetic phase for $U/W=4$, $J/W=1.5$, and $U'=U-2J$. Right panel: insulating ferromagnetic phase for $U/W=4$ and $J/W=0.5$. $\omega=0$ represents the Fermi energy.

phases. Note that this metal insulator transition is very different from the usual paramagnetic one, which appears in the Hubbard model at half filling as function of U. The MIT observed here between the ferromagnetic phases is rather due to a strong interorbital density-density interaction, which is responsible for driving the orbital ordering. As the latter introduces a doubling of the unit cell, the insulating solution is thus akin to the antiferromagnetic insulator. The usual intraorbital Hubbard interaction U plays a minor role in this transition.

It is worth noting that within a simplified two-site model representing the AB structure of the Néel state the antiferro-orbital situation wins over the orbitally homogeneous for all values of U' and J due to virtual hopping and the gain of Hund's exchange energy. It is thus the presence of the lattice which allows for smaller U' through an additional gain in kinetic energy the formation of the homogeneous metallic ferromagnet. In view of effects like colossal magneto resistivity it is an obviously interesting question, what influence external control parameters such as temperature and magnetic field will have when one is close to the phase transition. These questions are presently under investigation.

Another important aspect is the dependence of the phases upon doping. For the homogeneous ferromagnetic phase we already saw when discussing Fig. 2, that its filling can be varied smoothly. The dependency on the chemical potential of the orbital ordered ferromagnet, on the other hand, is dramatically different and can be seen in Fig. 6. The plot shows that for a critical chemical potential the filling of the system jumps from approximately $n=0.88$ to quarter filling $n=1$. At the same critical chemical potential also the polarization jumps from a nonpolarized phase to nearly fully polarized. In other words, there is a first-order transition between a paramagnetic phase with filling less than one and an orbitally ordered ferromagnetic state at quarter filling. Consequently the electronic system shows phase separation between these states and the precise physics will depend on additional interactions, such as long-range Coulomb interaction, or additional degrees of freedom such as the lattice. As already noted before, this appearance of phase separation is similar

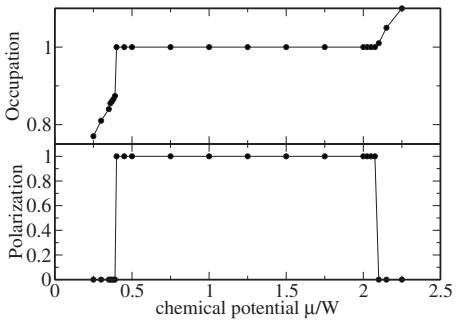

FIG. 6. Orbital ordered ferromagnetic insulator for $U=4W$, $J=W/2$, and $U'=U-2J$ as function of the chemical potential. The upper (lower) panel shows the occupation (polarization). Notice the jump in these quantities.

to what we find in the Hubbard model in the antiferromagnetic phase at half filling,[31,48–50] and thus seems to be a generic feature of the symmetry broken phases on an AB lattice. Note, however, that longer-ranged hopping can actually destroy this phase separation,[31] depending on the sign of the additional hopping and the type of doping.

In the region of large U', where the orbitally ordered ferromagnet is found, we were also able to stabilize an antiferromagnetic phase at quarter filling. As the system at quarter filling is dominated by ferromagnetic double exchange, one actually does not expect such a phase here. Like the orbitally ordered ferromagnet, this antiferromagnetic phase also exists only exactly at quarter filling. The spectral function and the doping dependence can be seen in Fig. 7. The spectral function shows that also this state is a perfect insulator. When trying to dope it we again find phase separation to a paramagnetic metal away from quarter filling. In order to find out which state is the thermodynamically stable one, we calculated the energy of both states. The result is that, as expected, the orbital ferromagnet has the lower energy, thus is the thermodynamically stable one. Looking at the different terms in the energy, the kinetic energy gives a larger decrease for the antiferromagnetic state than for the ferromagnetic state, while the interaction terms increase the energy of the antiferromagnet. Varying the parameters J and U', we always find the antiferromagnetic state having the higher energy.

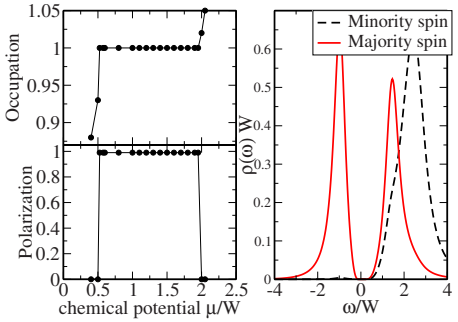

FIG. 7. (Color online) Antiferromagnetic insulator for $U=4W$, $J=W/2$, and $U'=U-2J$ as function of the chemical potential. The upper (lower) panel shows the occupation (polarization). Notice the jump in the properties. The right panel shows the spectral function.

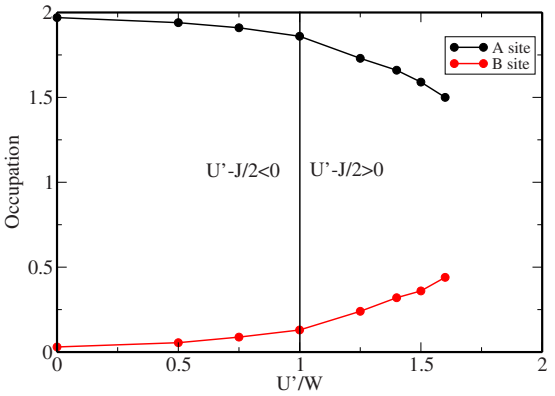

FIG. 8. (Color online) Occupation of neighboring sites in the charge ordered state for $J/W=2$. The interorbital interaction becomes repulsive for $U'/W>1$. The lines are meant as guide to the eye.

C. Charge ordering at quarter filling

For large Hund's coupling $J/2>U'$, the term $U'-J/2$ defining the interorbital density-density interaction becomes attractive. Although at first glance such a large Hund's coupling appears unphysical, one might have situations, for example Jahn-Teller coupling to phonons, which can lead to additional contributions to U', typically reducing it effectively. In this case such an attractive interaction can effectively be generated and the physics will change dramatically. The first thing one notes is that during a numerical calculation it becomes very difficult to stabilize fillings other than $n=2$ or 0. Inspired by this difficulty we investigated charge ordered phases in this parameter regime; and for sufficiently large Hund's coupling J it is indeed possible to stabilize a charge ordered state with alternating almost doubly occupied and nearly empty sites and an average occupation of $n=1$, see Fig. 8. Interestingly, this state seems to reach into the regime with $U' \gtrsim J/2$, already representing a repulsive interorbital interaction. If U' is increased further, this charge ordered state finally becomes unstable for $U'_c/W \approx 1.7$, i.e., we obtain a quarter-filled paramagnetic state. Note that we do not observe a vanishing order parameter but rather a jump as $U' \nearrow U'_c$, indicating a first order transition here, too. Another open point is how the charge ordered state connects to the magnetic phases present in this parameter region. As we have not yet been able to perform calculations allowing for both charge and magnetic order, we cannot tell whether there is a direct transition into one of the ferromagnetic phases rather than to the paramagnetic state. For the magnetic properties of the charge ordered state one may expect some kind of magnetic order between the half filled sites, which however requires larger unit cells to be used in the calculations. Besides magnetism, the charge density wave state is a perfect insulator, too, and again it is not possible to dope this state away from quarter filling.

IV. SUMMARY

In conclusion, we have analyzed the magnetic phase diagram of a two-orbital Hubbard model within DMFT and NRG. While around half filling the system behaves quite similar to the one orbital Hubbard model, there occurs an extended ferromagnetic phase for occupation $\langle n \rangle < 1.5$. Such a ferromagnetic phase cannot be observed for the one orbital case on a Bethe lattice with semielliptic DOS and is due to double exchange mechanism present in the two-orbital model. With increasing Hund's coupling J this ferromagnetic phase becomes more and more extended and finally can also be observed for occupation smaller than 1.

A particularly important point in the phase diagram is quarter filling, where we could observe four different ordered phases, and an especially interesting feature of the quarter-filled case is the presence of a metal insulator transition between two ferromagnetic states. The transition seems to be of first order and is driven by the interorbital density-density interaction U'. For low U' the ferromagnetic state is homogeneous and metallic. For large U', an orbital order can be observed in addition to the ferromagnetic one, which now is accompanied by an insulating behavior as the orbital order breaks translational symmetry similar to the Néel state at half filling.

Besides these ferromagnetic states, we also could stabilize an antiferromagnetic insulating and a charge ordered insulating state at quarter filling. The antiferromagnetic state exists in the same parameter region as the orbital ordered ferromagnetic state, but has a higher energy, i.e., will not be the thermodynamically stable one. The charge ordered state can be observed for rather large Hund's coupling J respectively reduced interorbital density interaction U'. The latter situation can for example be realized in the presence of Jahn-Teller phonons, which definitely play an important role in two-orbital systems with e_g symmetry. Thus, the inclusion of lattice degrees of freedom is a very important extension and presently under investigation.

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