Orbital-selective Mott transitions in the 2-band $J_z$-model: a high-precision quantum Monte Carlo study

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Using high-precision quantum Monte Carlo (QMC) simulations within the framework of dynamical mean field theory (DMFT), we show that the anisotropic degenerate two-orbital Hubbard model contains two consecutive orbital-selective Mott transitions (OSMTs) even in the absence of spin-flip terms and pair-hopping processes. In order to reveal the second transition we carefully analyze the low-frequency part of the self-energy and the local spectral functions. This paper extends our previous work to lower temperatures. We discuss the nature – in particular the order – of both Mott transitions and list various possible extensions.

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Introduction

Recently, the experimental discovery [1] of two consecutive orbital-selective metal-insulator transitions in the effective 3-band system Ca$_{2-x}$Sr$_x$RuO$_4$ triggered a cascade of papers also in the theoretical literature. The great interest in these “orbital-selective Mott transitions” can easily be understood. After initial LDA and DMFT [2], band structure [3, 4], and strong-coupling [5] calculations, it became clear that the occurrence of OSMTs in Ca$_{2-x}$Sr$_x$RuO$_4$ is a non-perturbative correlation phenomenon, which generalizes the famous concept of the classical “Mott transition” [6] to multi-band systems with inequivalent bands. The orbital-selective nature of the transitions also raises fundamental questions, such as, e.g., whether phase transitions in two subsystems merge or remain distinct, depending on the way these two subsystems are being coupled.

The microscopic model used in the literature to describe the OSMT phenomenon theoretically is the anisotropic degenerate two-orbital Hubbard model with [7,8,9,10,11,12] or without [13,14,15,16] spin-flip terms and pair-hopping in the Hamiltonian. For the model without these additional terms (the “$J_z$-model”) it was first believed [13,14] that only one transition exists at low temperatures, i.e., that the transitions which occur in the separate orbitals merge upon unison. Since two transitions clearly exist for the model with spin-flips and pair-hopping (the “$J$-model”) it was believed [8] that these additional terms cause the two transitions of the subsystems to remain distinct and, hence, make a fundamental difference. Here we show, extending previous work in [15], that the $J_z$-model does, in fact, also contain two distinct OSMTs. In this manner we establish the $J_z$-model as a minimal model for the description of the OSMT phenomenon.

The Hamiltonian of the $J_z$-model,

$$H = - \sum_{(ij)\mu\sigma} t_{ijm} c_{i\mu\sigma}^\dagger c_{j\mu\sigma} + U \sum_{im} n_{im\uparrow} n_{im\downarrow} + \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z) n_{i\sigma\sigma'} n_{i\sigma'\sigma'},$$

describes hopping between nearest-neighbor sites $i, j$ with amplitude $t_{ijm}$ for orbital $m \in \{1, 2\}$, intra- and interorbital Coulomb repulsion parametrized by $U$ and $U'$, respectively, and Ising-type Hund’s exchange

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coupling $J_z$; $n_{im\sigma} = c_{im\sigma}^\dagger c_{im\sigma}$ for spin $\sigma \in \{\uparrow, \downarrow\}$. As usual, we consider this model with $U' = U - 2J_z$. Specifically, our DMFT (QMC) results for this model, to be presented below, were calculated using semi-elliptic densities of states with full bandwidths $W_1 = 2$, $W_2 = 4$, for the “narrow” and “wide” band, respectively, and interaction parameters $J_z = U/4$, $U' = U/2$.

It is important to emphasize that high-precision in the QMC simulations is essential for the investigation of OSMTs, since the signals of in particular the second transition are rather subtle and can easily be missed. In [16] we showed that our QMC results for, e.g., quasi-particle weights, have relative errors of $O(10^{-2})$ even near the critical interactions $U_{c1} \approx 2.0$ and $U_{c2} \approx 2.5$ for the first and second transition, respectively. This is an improvement of up to two orders of magnitude compared to previous QMC results [13] [14]. The high precision in our simulations is (at least in part) due to the reduction of the discretization error achieved by complementing QMC data with a high-frequency expansion of the self-energy [17] [18].

**Results** In the following, we present QMC results for the $J_z$-model with band widths and interaction parameters as stated before. We briefly discuss one of the primary criteria used in Ref. [15] for detecting the two OSMTs in Fig. 1 (cf. also inset of Fig. 5) before turning to new results.

As shown in Fig. 1, a low-frequency analysis of the self-energies associated with both bands clearly reveals the orbital-selective character of the first transition at $U_{c1} \approx 2.0$ (associated with the narrow band) and the existence of a second transition (associated with the wide band) at $U_{c2} \approx 2.5$: for $U \approx U_{c1}$, only the narrow band develops a singularity the weight of which (filled symbols) increases approximately linearly with $U$. In contrast, the corresponding weight for the narrow band remains zero (numerically) up to $U \approx U_{c2}$; above this point, again, a linear increase with $U$ is observed. Note that temperature dependencies are hardly visible; however, the kink at $U_{c2}$ becomes slightly sharper with decreasing $T$. The extraction of the weights shown in the main panel from fits to products $\omega \Sigma(\omega)$ is illustrated in the inset to Fig. 1.

Metal-insulator transitions may also be identified from discrete estimates of the quasiparticle weight $Z \approx [1 - \text{Im} \Sigma(i\pi T)/(\pi T)]^{-1}$ (even though this observable is somewhat problematic [15] [16]): kinks in $Z$, most markedly for the narrow band, reveal a transition at $U_{c1} \approx 2.0$ in the inset of Fig. 2; a second transition for $U_{c2} \approx 2.5$ would become apparent at higher resolution. The main panel of Fig. 2 shows a

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**Fig. 1** Low-frequency analysis of the self-energy. Main panel: weight of singularity at $\omega = 0$ for narrow/wide band (filled/open symbols) as extracted from polynomial fits to the product $\omega \Sigma(\omega)$ [shown in inset for $T = 1/32$ and $U = 2.8, 2.6, 2.4, 2.2, 2.0, 1.8$ (top to bottom)].

**Fig. 2** Quasiparticle weight $Z = m/m^*$. Inset: $Z$ for wide/narrow band (open/filled symbols) across OSMTs at $U_{c1} \approx 2.0$ and $U_{c2} \approx 2.5$ for $T = 1/40$. Main panel: detailed study of first transition at $U_{c1}$ reveals hysteresis (i.e. a 1st order transition) only for $T < T^* \approx 0.02$. 
close-up of $Z$ near $U_{c1}$ for a range of temperatures. Evidently, the observables vary continuously with $U$ for $T = 1/32$ and $T = 1/40$; only for $T = 1/50 = 0.02$, we find first traces of stable coexistence, signaling a first-order transition. Thus, we estimate $T_{c1}^* \approx 0.02$ which agrees with recent independent exact diagonalization (ED) results [22], but is much lower than earlier QMC and ED estimates (of $T_{c1}^* \approx 0.038 [14]$ and $T_{c1}^* \gtrsim 0.03 [23]$, respectively).

Valuable insight into the nature of phases and transitions can be gained from the spectral functions, shown for the narrow and wide band in the left and right hand panel of Fig. 3 respectively. The narrow-band spectra show typical Fermi-liquid behavior: the quasiparticle peak becomes narrow before it decays and, finally, a gap appears for $U \gtrsim 2.05$. In contrast, the wide-band quasiparticle peak remains wide, but develops a dip near the Fermi energy before a full gap appears at $U \approx 2.6$. The density of states at the Fermi energy, shown in the inset of Fig. 3, further illustrates the OSMT scenario: At $U_{c1} \approx 2.0$ the narrow band undergoes a metal-insulator transition while the wide band is hardly affected; the latter becomes insulating only above $U_{c2} \approx 2.5$.

Summary and Discussion We have shown that, contrary to previous statements in the literature, the two-band Hubbard model with distinct band widths $W_2 = 2W_1$ and interaction parameters $U, U' = U/2, J_z = U/4$ does in fact describe the occurrence of orbital-selective Mott transitions, as seen experimentally in the Ca$_{2-x}$Sr$_x$RuO$_4$-system. This “$J_z$-model” can therefore be considered as a minimal model for the theoretical description of OSMTs. We also showed that the method used in this paper, viz. high-precision QMC calculations at finite temperatures, is well-suited for the study of OSMTs, provided the correct high-frequency behavior of the self-energy is implemented with care and full convergence in the DMFT cycle is established. The observables studied in this paper, revealing two consecutive Mott transitions, are the spectral functions, the low-energy behavior of the self-energy, and the quasiparticle weights.

The question concerning the order of the transitions at $U_{c1} \simeq 2.0$ and $U_{c2} \simeq 2.5$ is both interesting and important. The results presented here suggest that physical quantities, like the quasiparticle weights, display a jump at sufficiently low temperatures for $U = U_{c1}$, so that the first transition is likely of first order below $T_{c1}^* \approx 0.02$. In contrast, these observables are continuous for the $J_z$-model at $U = U_{c2}$, as expected for a second-order transition. At present it would be premature, however, to make definite statements concerning the second transition, because high-precision QMC calculations are at present difficult (since computationally costly) in the relevant low-temperature regime and also because it is numerically difficult.

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to distinguish a real second-order transition at $T > 0$ from a narrow cross-over, eradiating possibly from a $T = 0$ quantum critical point. In spite of these numerical uncertainties, we wish to point out that the occurrence of a first-order transition at $U_{c1}$ and a second-order transition at $U_{c2}$ are physically plausible. A first-order transition for the narrow band at $U_{c1}$ is exactly what one expects on the basis of experience with the Mott transition in the single-band Hubbard model [6, 19, 20, 18]. The orbital-selective phase between $U_{c1}$ and $U_{c2}$ is characterized by itinerant electrons in the wide band, interacting with immobile (localized) electrons in the narrow band, which is essentially Falicov-Kimball physics. Since the metal-insulator transition in the symmetric spinless Falicov-Kimball model is of second order (Hubbard-III-like), the same scenario could apply to the $J_z$-model at $U_{c2}$. Our results further show non-Fermi-liquid behavior of the wide band for $U_{c1} < U < U_{c2}$, which is again to be expected on the basis of the Falicov-Kimball analogy. The connection to the Falicov-Kimball model was recently also pointed out by Biermann et al. [21]; for a discussion of non-Fermi-liquid physics cf. also [22].

As an outlook, we discuss several extensions of the present work. Clearly, since the transition temperature at $U_{c1}$ appears to be rather low ($T_{c1}^* \approx 0.02$), it is important to obtain results at even lower temperatures than were considered in this paper. The inclusion of spin flips remains an important problem. Since the experimental system Ca$_{2-x}$Sr$_x$RuO$_4$ has three bands, two of which are physically equivalent, it may be worthwhile to study the OSMTs in a real 3-band-model. For comparison with the experimental situation, additional hybridization between the bands needs to be taken into account; first results [10] suggest that hybridization influences the OSMT dramatically. Since anisotropy is by definition important for the OSMT, it is only consistent to take also orbital-dependent interaction strengths into account. Since the experimental system is an antiferromagnetic insulator for small doping ($x \lesssim 0.2$), it is important to extend the present work to include also magnetic phases. In conclusion, the study of OSMTs will doubtlessly remain exciting, yielding unexpected important results in the months to come.

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