Orbital-selective Mott transitions in two-band Hubbard models

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Abstract

The anisotropic two-orbital Hubbard model is investigated at low temperatures using high-precision quantum Monte Carlo (QMC) simulations within dynamical mean-field theory (DMFT). We demonstrate that two distinct orbital-selective Mott transitions (OSMTs) occur for a bandwidth ratio of 2 even without spin-flip contributions to the Hund exchange, and we quantify numerical errors in earlier QMC data which had obscured the second transition. The limit of small inter-orbital coupling is introduced via a new generalized Hamiltonian and studied using QMC and Potthoff’s self-energy functional method, yielding insight into the nature of the OSMTs and the non-Fermi-liquid OSM phase and opening the possibility for a new quantum-critical point.

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1. Introduction

Recently, the suggestion [1] that the two consecutive phase transitions experimentally observed [2] in Ca$_{2-x}$Sr$_x$RuO$_4$ should be interpreted as “orbital-selective Mott transitions” (OSMTs) sparked a cascade of related theoretical papers (see [3] and references therein).

Microscopic studies of OSMTs usually consider the 2-band Hubbard model $H = H_1 + H_2 + H_3$, where

$$H_1 = - \sum_{(i,j)m} t_m c_{i m \sigma}^\dagger c_{j m \sigma} + U \sum_{im} n_{im\uparrow} n_{im\downarrow},$$

$$H_2 = \sum_{i \sigma'} (U' - \delta_{\sigma' \sigma} J_z) n_{i \sigma} n_{i \sigma'},$$

include hopping between nearest-neighbor sites $i,j$ with amplitude $t_m$ for orbital $m \in \{1, 2\}$, 

intra- and inter-orbital Coulomb repulsion parametrized by $U$ and $U'$, respectively, and Ising-type Hund’s exchange coupling; $n_{im\sigma} = c_{im\sigma}^\dagger c_{im\sigma}$ for spin $\sigma \in \{\uparrow, \downarrow\}$. In addition,

$$H_3 = \frac{1}{2} J_z \sum_{i m} c_{i m\uparrow}^\dagger \left( c_{i m\uparrow} c_{i m\downarrow} + c_{i m\downarrow}^\dagger c_{i m\uparrow} \right) c_{i m\uparrow},$$

contains spin-flip and pair-hopping terms (with $\downarrow \equiv 2, \uparrow \equiv 1$ etc.). As in [3], we refer to $H_1 + H_2 + H_3$ with the isotropic coupling $J_z = J_{\perp}$ as the $J$-model and to the simplified Hamiltonian $H_1 + H_2$ as the $J_z$-model; unless noted, $U' = U/2, J = U/4$ so that $U' + 2J = U$.

Early theoretical studies suggested that the expected 2 distinct OSMTs occur only in the full $J$ model [4], but not in the Ising type $J_z$-model [5,6]. Thus, it seemed as if spin-flip and pair-hopping terms were essential ingredients to orbital-selective physics. However, this is not actually the case, as shown in a low-frequency analysis of high-precision QMC data [3] in Fig. 1a: a singularity develops at $\omega = 0$ for $U_{c1} \approx 2.0$ in the narrow-band self-energy, but only at $U_{c1} \approx 2.5$ in the wide-band self-energy (with linear increase for $U > U_{c1/2}$). Corresponding spectra (Fig. 1b) illustrate the characteristics of the 3 distinct phases.

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Fig. 2. a) QMC estimates of quasiparticle weights $Z$ at $T = 1/32$: a) high-precision data [3] (circles, crosses) clearly shows kinks at $U_{c1} \approx 2.0$; b) suitable analysis reveals a second kink at $U_{c2} \approx 2.5$. The second transition is lost in the noise of earlier data [5] (squares) with errors exceeding 100% at both transitions (c).

Fig. 3. Quasiparticle weights for generalized two-orbital model: at $T = 1/40$, the wide-band transition remains first order (with hysteresis) for small enough inter-orbital coupling $\alpha \lesssim 0.2$.

Discrete estimates $Z = [1 - \text{Im} \Sigma (i\pi T)/(\pi T)]^{-1}$ for the quasiparticle weight clearly show (only) the narrow-band transition (Fig. 2a); a second (wide-band) transition is visible as kink only in high-precision QMC data (circles, crosses) and after adding a linear term (Fig. 2b). Possible signals from this transitions cannot be distinguished from numerical errors in earlier QMC data [5] (squares) since they exceed 100% at both transitions (Fig. 2c).

2. Limit of small inter-orbital coupling

Clearly, the resolution of two orbital-selective Mott transitions with critical interactions differing by only about 20% is a very challenging task, in particular at temperatures attainable using QMC. In this situation, much insight can be gained by abandoning the constraint $U' + 2J = U$ fulfilled in nearly all earlier studies and instead studying the limit of small inter-orbital coupling. Hence, we consider $H = H_1 + \alpha H_2$ with $0 \leq \alpha \leq 1$ so that $\alpha = 0$ corresponds to uncoupled orbitals and $\alpha = 1$ to the case studied previously.

It is a priori clear, that for $\alpha = 0$ each orbital should undergo a usual Mott transition at an interaction determined by the corresponding bandwidth ($W = 2$ for the narrow, $W = 4$ for the wide band); note however, that even in this case the QMC results for both orbitals have no scaling relation at fixed $T > 0$. This is seen in Fig. 3: For $\alpha = 0$, a large hysteresis region appears in the wide-band quasiparticle weight (uppermost, grey line) while only a single coexistence point is resolved for the narrow band (at $T = 1/40$). Very importantly, the wide-band transition evidently remains first order at small, but significant inter-orbital coupling ($\alpha = 0.1$, $\alpha = 0.2$). It may be expected that the first-order range (in $\alpha$) increases at lower temperatures which suggests that the wide-band OSMT might be very weakly first order even at $\alpha = 1$. However, the alternative of a quantum phase transition at some critical value $\alpha = \alpha_c$ is equally interesting and warrants further investigation.

3. Nature of orbital-selective Mott phase

As shown above, the (discretely estimated) quasiparticle weight $Z$ is not well suited for detecting the second OSMT. In fact, it is even misleading in the OSM phase: as seen in Fig. 4a, $Z_{\text{wide}}$ is nearly constant as a function of $T$ in the metallic Fermi-liquid phase ($U = 2.0$). However, this observable decays to 0 for $T \to 0$ in the OSM phase. Naively, one might conclude that the OSM phase becomes indistinguishable from the insulating phase for $T = 0$. However, Fig. 4b proves that this is not the case: the self-energies are practically $T$-independent both in the metallic and in the OSM phase [with agreement between QMC results for different $T$ and self-energy functional theory in dynamical impurity approximation (DIA)]; thus, the $T$ dependence in $Z_{\text{wide}}$ is an artifact of the discrete approximation. The non-Fermi-liquid character of the wide band in the OSM phase is clearly seen as the finite limit of $\text{Im} \Sigma$ for $\omega \to i0^+$.

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