Metal insulator transitions driven by local Coulomb interactions are among the most fascinating phenomena in condensed matter physics. They occur in a large variety of transition metal compounds. Most of these strongly correlated materials consist of valence bands derived from electronic d shells where intra- and inter-orbital Coulomb interactions are equally important and where the crystal structure splits the valence bands into narrow and wide subbands. A fundamental question is whether these systems exhibit a common Mott transition, implying all subbands to be either metallic or insulating, or successive orbital dependent transitions, implying a coexistence region with metallic and insulating behavior present in different subbands. Using the dynamical mean field theory, we show that inter-orbital Coulomb interactions lead to a single Mott transition. Nevertheless, the subbands exhibit more or less strongly correlated excitation spectra in the metallic phase and different band gaps in the insulating phase.

A hallmark of strongly correlated materials is their geometrical, electronic and magnetic complexity. The valence bands typically involve oriented electronic orbitals, giving rise to a variety of highly anisotropic properties. For instance, the layer perovskite Sr$_2$RuO$_4$ consists of a wide, two-dimensional $d_{xy}$ band coexisting with narrow, nearly one-dimensional $d_{z^2,xy}$ bands. This system exhibits unconventional p-wave superconductivity, but iso-electronic replacement of Sr by Ca induces a Mott transition to an antiferromagnetic insulator. Similar splittings into different subbands occur in the classic Mott insulators VO$_2$ and V$_2$O$_3$ in both the low-temperature insulating (monoclinic) and high-temperature metallic (rutile, corundum) phases, in layered organic superconductors, fullerenes, and many other compounds.

The nature of the paramagnetic metal insulator transition in a multi-band environment involving narrow and wide subbands is not yet understood; in particular, it is not clear whether all bands undergo a common transition at the same critical Coulomb energy or whether different subbands generate transitions at successive critical energies. In the first scenario narrow subbands force wide subbands to become more strongly correlated and the more pronounced metallicity of wider subbands makes narrow bands less correlated than in the isolated case. The critical Coulomb energy $U_c$ of the interacting system lies between the critical $U_{ci}$ of the isolated subbands. Coexistence of metallic and insulating behavior in different subbands does not occur. In the second scenario the different relative importance of Coulomb correlations in subbands of different widths gives rise to separate Mott transitions and to coexistent metallic and insulating behavior in different subbands. In this case the one-electron properties imposed by the different band widths remain a determining factor for the system’s excitation spectrum and are not entirely superseded by correlations.

While local Coulomb interactions in multi-band systems have been investigated previously, most studies treated the special ‘isotropic’ case of identical orbitals where the question of one or several Mott transitions does not arise. Here we consider the opposite ‘non-isotropic’ situation where the multi-band system consists of different subbands. In the absence of inter-orbital Coulomb interactions these bands would exhibit Mott transitions at different critical energies $U_{ci}$. As shown below, the striking consequence of inter-orbital interactions is to enforce one common metal insulator transition for all subbands at the same critical $U_c$. Remarkably, however, in the joint metallic region different subbands reveal excitation spectra with varying correlation signatures. Similarly, the insulating phase exhibits a ‘multi-gap’ spectrum, in close analogy to the $\sigma$- and $\pi$-type superconducting gaps observed in the quasi-two-dimensional compound MgB$_2$.

Let us consider the paramagnetic metal insulator transition in a two-band Hubbard model with narrow and wide subbands. These might represent, for instance, the $t_{2g}$ orbitals of a layer-perovskite material or of VO$_2$. For illustrative purposes these bands are assumed to be half-filled and to have elliptical densities of states $\rho_1(\omega)$ of widths $W_1 = 2\,eV$ and $W_2 = 4\,eV$. Single-band systems of this type have been investigated extensively in the past and their metal insulator transitions are rather well understood. To account for Coulomb correlations we use the dynamical mean field theory (DMFT) in combination with the multi-orbital Quantum Monte Carlo (QMC) method. The quantum impurity problem is solved at finite temperature $T$ for various intra- and inter-orbital Coulomb energies $U$ and $U' = U - 2J$, where $J$ is the Hund’s rule exchange integral.

Two criteria are employed to determine the stability of the Fermi liquid state as a function of Coulomb energy. First, we calculate the subband quasi-particle weights $Z_i = 1/(1 - \partial\Re \Sigma_i(\omega)/\partial\omega|_{\omega=0})$, where the derivative of the real part of the self-energy component $\Sigma_i(\omega)$ is approximated by $\Im \Sigma_i(i\omega_0)/\omega_0$ with $\omega_0 = \pi/\beta = \pi k_B T$ the first Matsubara frequency. The second criterion is obtained from the imaginary-time Green’s functions at $\tau = \beta/2$: $G_i(\beta/2) = \int d\omega F(\omega) \Im G_i(\omega)/\pi$, where
\[ F(\omega) = \frac{0.5}{\cosh(\beta\omega/2)} \] is a distribution of width \( w = 4 \ln(2 + \sqrt{3})/\beta \) centered about the Fermi level. While \( Z_i \) specifies the quasi-particle weight of the \( i \)th subband at \( E_F \), \( G_i(\beta/2) \) represents the integrated spectral weight within a few \( k_B T \) of \( E_F \), i.e., it includes low-lying excitations. Since \( \Sigma_i(\omega_n) \) and \( G_i(\tau) \) are derived directly from the QMC calculation \( Z_i \) and \( G_i(\beta/2) \) are available without having to evaluate the real-frequency spectral distributions \( \text{Im} G_i(\omega) \). Below we present normalized quantities \( \tilde{G}_i(\beta/2) = \tilde{G}_i(\beta/2) / \tilde{G}_i(\beta/2) = 1 \) in the non-interacting limit.

Figure 1 shows the variation of \( Z_i \) and \( G_i(\beta/2) \) as a function of \( U \) for \( T = 125 \text{ meV} \). The exchange integral is \( J = 0.2 \text{ eV} \). Evidently the quasi-particle weights near \( E_F \) diminish as a result of Coulomb correlations. At a given \( U \), however, \( Z_1 \) and \( \tilde{G}_1 \) in the non-isotropic \( W_1, W_2 \) system are larger than in the degenerate \( W_1, W_1 \) case. Similarly, \( Z_2 \) and \( \tilde{G}_2 \) in the \( W_1, W_2 \) system are smaller than in the \( W_2, W_2 \) case. Thus, as a consequence of inter-orbital interactions the narrow (wide) subband is less (more) correlated than in the isotropic case.

Since \( G_i(\beta/2) \) represents the spectral weight within several \( k_B T \) of \( E_F \) its reduction at small \( U \) is weaker than that of \( Z_i \), while in the critical regions its decay is more abrupt. Close to the metal-insulator transitions \( Z_i \) and \( G_i \) show a rounding off caused by the finite temperature and by critical slowing down. Within this slight uncertainty \( Z_i \) and \( G_i \) yield consistent critical Coulomb energies: \( U_{c1} \approx 3.0 \text{ eV} \) for the narrow two-band system, \( U_{c2} \approx 6.1 \text{ eV} \) for the wide two-band system, and \( U_c \approx 4.8 \text{ eV} \) for the mixed system.23

The key point of these results is the fact that the system involving narrow and wide subbands exhibits a single Mott transition at an intermediate \( U_c \) such that \( U_{c1} < U_c < U_{c2} \). At small \( U \) correlations reduce the quasi-particle weight in the narrow subband much more rapidly than in the wide band. For \( U > U_c/2 \), however, \( Z_1 \) and \( Z_2 \) begin to converge again and decrease to zero spectral weight at the same \( U_c \). The same behavior is shown by the integrated weights \( \tilde{G}_i(\beta/2) \). There is no evidence for a coexistence of insulating and metallic behavior in different subbands.23 On the other hand, since \( Z_1 < Z_2 \) and \( \tilde{G}_1 < \tilde{G}_2 \) for \( U < U_c \), the narrow band is always more strongly correlated than the wider counterpart. Analogously, the insulating phase exhibits two excitation gaps (see below).

Multi-band QMC calculations at lower temperatures (\( T = 62 \text{ meV} \) and 31 meV) confirm the picture discussed above. To verify that the same conclusion holds also in the low temperature limit we have performed analogous two-band calculations at \( T = 0 \) within the self-consistent iterated perturbation theory (IPT), where the self-energy is calculated at real frequencies within second-order perturbation theory. The results for the quasi-particle weights \( Z_i \) are shown in Fig. 2. They are consistent with the scenario for \( T > 0 \): The isotropic two-band systems have widely different critical Coulomb energies: \( U_{c1} \approx 2.3 \text{ eV} \) and \( U_{c2} \approx 4.3 \text{ eV} \). In contrast,
of the different temperatures.

Although inter-orbital Coulomb interactions lead to a common metal insulator transition in the narrow and wide subbands, their excitation spectra differ qualitatively both in the metallic and insulating phases. This is illustrated in Fig. 3 where we plot quasi-particle distributions derived using the Maximum Entropy method. For $U < U_c$, both bands are metallic. The narrow band spectrum $N_1(\omega)$, however, is more strongly correlated than $N_2(\omega)$ for the wider band: The spectral weight at $E_F$ is much reduced and the Hubbard peaks are more pronounced. Similarly, in the insulating phase the excitation gap of the narrow band is larger than that of the wide band. Note that the $W_1, W_1$ system at $U = 4\,\text{eV}$ is already insulating, while the $W_2, W_2$ system is much less correlated than the $N_2(\omega)$ spectrum shown in Fig. 3(a). Conversely, at $U = 6\,\text{eV}$ the $W_1, W_1$ system is far in the insulating range, whereas the $W_2, W_2$ system is close to its metal insulator transition.

These predictions can be tested using angle resolved photoemission spectroscopy. In the metallic phase of layered perovskites, for example, the $d_{xy}$ and $d_{xz/yz}$ subbands should exhibit coherent peaks of different spectral weights as well as different incoherent satellite features. At $U_c$ the coherent peaks should vanish simultaneously. In the insulating phase, the subbands should exhibit different band gaps and Hubbard bands.

For illustrative purposes we have considered the special case of half-filled, symmetric subbands. The consistency of the picture discussed here with the results obtained for $\text{Ca}_2-\text{Sr}_x\text{RuO}_4$ suggests that the same conclusion holds for non-symmetric multi-band systems. In particular, it should be valid for the Mott insulators $\text{VO}_2$ and $\text{V}_2\text{O}_3$ and for other transition metal compounds.

Acknowledgements

I am grateful to A. Bringer for discussions and to O. Gunnarsson and D. Vollhardt for comments. I also like to thank A. Lichtenstein for the DMFT-QMC code.

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