1 Introduction

Dynamical Mean-Field theory (DMFT) has proven to be a fantastic tool to study the Hubbard model and Mott-Hubbard transitions. Still, the nature of Mott-Hubbard transitions is complex as we get away from the most simple models. Notably, in the years 2003 to 2005, a controversy was sparked regarding the existence of Orbital-Selective Mott Transitions (OSMTs). Indeed, in many transition metal oxides, multiple bands typically cross the Fermi surface, notably the t_{2g} or e_g orbitals, and different bandwidths for different bands might give rise to multiple transition for each bands. This is the case for the cuprate $Ca_{2-x}Sr_xRuO_4$ which undergoes a Mott transition as x is increased from 0 [1].

The model considered in this paper will be the case of two bands, one narrow ($W = 2eV$) and one wide band ($W = 4eV$). The Hamiltonian used will be the Hubbard hamiltonian with interband coupling accounting for Hund's exchange :

$$\begin{aligned} H = &- \sum_{\langle i,j\rangle m\sigma} t_m \hat{c}^\dagger_{im\sigma}\hat{c}_{jm\sigma} \\ &+ U\sum_{im\sigma}\hat{n}_{im\uparrow}\hat{n}_{im\downarrow} + \sum_{i\sigma\sigma'}\left(U' - \delta_{\sigma\sigma'}J_z\right)\hat{n}_{i1\sigma}\hat{n}_{i2\sigma'} \\ &+ \frac{J_\perp}{2}\sum_{im\sigma}\hat{c}^\dagger_{im\sigma}\left(\hat{c}^\dagger_{i\bar{m}\bar{\sigma}}\hat{c}_{im\bar{\sigma}} + \hat{c}^\dagger_{im\bar{\sigma}}\hat{c}_{i\bar{m}\bar{\sigma}}\right)\hat{c}_{i\bar{m}\sigma} \end{aligned}$$

This model takes into account single-band Coulomb repulsion with the term in U, interband repulsion with $U' = U - 2J_z$ and Hund's exchange may be kept asymmetric (J_z model) or simplified with $J_z = J_{perp} = J$ if the system is invariant under spin rotation (J model). Sum indices denote sites (i, j), band ($m = 1, 2$) and spin ($\sigma = \uparrow, \downarrow$) with bars indicating the opposite state for the two states variables.

Initial results from Liebsch refuted the existence of OSMT for the J_z model using a DMFT method with Quantum Monte-Carlo (QMC) solver at finite temperature [2] [3]. However, multiple papers later contradicted Liebsch's results and found an OSMT, first Koga et al. using DMFT with exact diagonalisation (ED) at zero temperature and the full J model [4], then Knecht et al. using DMFT with an improved QMC solver attempting to get rid of the sign problem at low temperature [5], using the same J_z model asq Liebsch. Finally Arita and Held also found an OSMT using projective QMC (PQMC) to tackle the J model at zero temperature [6].

2 Methods

Our goal in this paper is to use DMFT with a QMC solver to clarify the controversy and ensure the two-band Mott transition predictions is well understood and well described with current methods. To that end, we choose to study the full J model, which supposedly encompasses the full effects of correlation, and is also more interesting as it has only been studied at 0 temperature, contrary to the Jz model. In the Hamiltonian, t_m is set to 1 eV to set the energy scale. The parameters are chosen in accordance with previous papers on the matter, with the value of U variable and the ratios $J = U/4$ and $U' = U - 2J = U/2$ fixed ; additionally the two bands are set with bandwidths $W_1 = 2eV$ and $W_2 = 4eV$ in an elliptical density of states given by $\rho_i(\epsilon) = \frac{4}{\pi W_i}\sqrt{1 - 4\epsilon^2/W_i^2}$, and taken at half filling. Finally temperature is set to $\beta = \frac{1}{40}eV$, about room temperature.

In a Mott transition, the system undergoes a phase transition between a disordered phase for $U << t$, where the system is a conductor, and an ordered phase for $U >> t$, where the Coulomb repulsion prevents electron hopping and the system becomes an insulator. The difference between the two phases is striking when looking at the spectral function. In the insulating phase, all the spectral weight is contained in two lobes separated by a (Mott) gap. The non zero quasi-particle weight at zero frequency is a signature of the conductive phase: there are available states right above the last filled one and therefore no gap between the occupied and unoccupied states. Hence, to characterize the Mott transition, the parameter of choice is the quasi-particle weight at the Fermi energy, obtained from the self-energy :

$$Z_i = \frac{1}{1 - \frac{\partial}{\partial\omega}\mathrm{Re}(\Sigma_i)\Big|_{\omega=0}}$$

3 Results

The quasiparticle weight is plotted on Fig. **??**. The graph unambiguously shows an OSMT, with the narrow band becoming insulating at $U_{c1} \approx 2.1$ and the wide band at $U_{c2} \approx 3.1$. These results are to be compared with that of Koga's paper and Arita's paper, which show respectively $U_{c1} \approx 2.6, U_{c2} \approx 3.5$ and $U_{c1} \approx 2.6$

Overall, our results are close to but lower than that cited above. This is in good agreement with theory, predicting that the critical U at which transition occurs goes down as temperature is increased.

		J_z model		J model	
Author	T (eV)	U_{c1} (eV)	U_{c2} (eV)	U_{c1} (eV)	U_{c2} (eV)
Liebsch, 2004	1/32	2.5	2.5		
Koga et al., 2003	0			2.6	3.5
Knecht et al., 2005	1/40, 1/32	2.1	2.6		
Arita, Held, 2005	0			2.6	
Our results	1/40			2.1	3.1

Table 1: Table comparing numerical values for Mott transitions. Liebsch's first paper is omitted as the parameters used were too different. Our results are

4 Conclusion

Acknowledgements

References

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