

# 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  $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$  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 :

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

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. 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.

To characterize the Mott transition, the parameter of choice is the quasi-particle weight, obtained from the self-energy :

$$Z_i = \frac{1}{1 - \left. \frac{\partial}{\partial \omega} \Re(\Sigma_i) \right|_{\omega=0}}$$

## 3 Results

## 4 Conclusion

## Acknowledgements

## References

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