

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 ($W = 2\text{eV}$) and one wide band ($W = 4\text{eV}$). The Hamiltonian used will be the Hubbard hamiltonian with interband coupling accounting for Hund's exchange :

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

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 $J_z = J_{\text{perp}} = J$ 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

- [1] S. Nakatsuji and Y. Maeno. Quasi-two-dimensional mott transition system $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$. *Physical Review Letters*, 84(12):2666–2669, March 2000.
- [2] A. Liebsch. Mott transitions in multiorbital systems. *Physical Review Letters*, 91(22), November 2003.
- [3] A. Liebsch. Single mott transition in the multiorbital hubbard model. *Physical Review B*, 70(16), October 2004.
- [4] Akihisa Koga, Norio Kawakami, T. M. Rice, and Manfred Sigrist. Orbital-selective mott transitions in the degenerate hubbard model. *Physical Review Letters*, 92(21), May 2004.
- [5] C. Knecht, N. Blümer, and P. G. J. van Dongen. Orbital-selective mott transitions in the anisotropic two-band hubbard model at finite temperatures. *Physical Review B*, 72(8), August 2005.

- [6] R. Arita and K. Held. Orbital-selective mott-hubbard transition in the two-band hubbard model. *Physical Review B*, 72(20), November 2005.