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.

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

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

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.

4 Conclusion

Acknowledgements

References

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