

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 :

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

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

3 Results

4 Conclusion

Acknowledgements

References

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