March 3, 2025

Response to Referee 3

The authors present the solution (one-particle spectral function, self-energy and uniform susceptibility) of the three-band Emery model within the single-site DMFT approximation. In this model the electrons in the oxygen p-orbitals are treated as non-interacting and only the d-d onsite repulsion is taken into account. The DMFT approximates the solution by neglecting dynamical nonlocal correlations, which in this case means correlations beyond the unit cell. The parameters of the Emery model are adapted to describe the cuprate superconductors as in earlier cluster DMFT studies of Refs. 34 and 35. More precisely, one set of parameters is used. The one-particle spectra are discussed and compared directly with the one-band Hubbard model (also computed by the authors and placed in the Appendix) and indirectly with earlier cluster studies. The lack of momentum dependence in the self-energy and hence absence of the pseudogap is addressed and at the one-particle level the deficiencies (and also strengths) of DMFT carefully addressed. The authors then present two-particle calculations on the example of static uniform susceptibility, computed by performing computations at finite magnetic field. The numerical results are then compared to the experimental measurements of the Knight shift and (in the Appendix) to the one-band Hubbard model in DMFT as well as to the asymmetric dimer toy model. They find that the asymmetric dimer represents the qualitative temperature dependence of the susceptibility much better than the DMFT calculation for the one-band Hubbard model, which the authors assign to the singlet formation captured well by the dimer or by the Emery model (even in DMFT), but apparently not in the DMFT for the one-band Hubbard model. The single-site DMFT calculations are thought of as a starting point for a future DΓA study of the Emery model.

I find already the DMFT results interesting and certainly deserving publication. What I miss in the current version of the manuscript is a thorough discussion of two-particle properties as captured or not captured by DMFT. It is not clear to me why the uniform susceptibility is the correct quantity to represent the Knight shift in place of the local susceptibility. The authors should explain if this is related to the fact that the computational method used gives better results for uniform susceptibility, because it can be computed directly as a derivative and not from the correlation function (which I suspect to be the case), or to the actual way the experiments are performed. In case the authors address this point in detail, I recommend the paper for publication.

Response: We thank the Referee for their comments, their judgement that our results are *"interesting"*, and their support for publication in SciPost Physics after the raised issues have been clarified.

Requested Changes ("Minor Points")

1. I would appreciate a justification of the choice of the value of the onsite repulsion. Do the authors expect the results to depend on the precise value?

   Response: All parameters for the model (hopping and interaction) were taken from Refs. 34 (Weber et al. 2012) and 35 (Kowalski et al. 2021). They have been derived/estimated by means of downfolding techniques of ab initio DFT results. These preliminary works found that an interaction value of U_{dd} in the range of 8-10 eV and J around 1 eV reproduces key

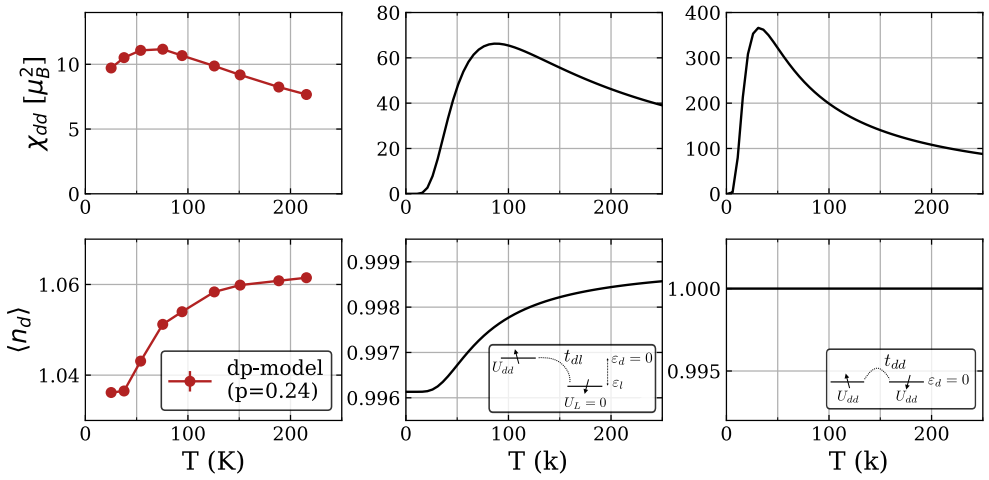

Figure 1:

experimental observables, such as the charge transfer gap, best. We now make this choice clearer in the revised version. While the quantitative results would surely depend on the specific U value, the overall doping and temperature trends we find in the susceptibility are - on a qualitative level - completely robust.

2. Optional: A third plot in Fig. 6 with the d-only spin susceptibility (if data are available for the relevant temperatures) could make the argumentation stronger.

Response: As shown in Fig. 1 a symmetric dimer model with U on both sides would also lead to singlet fluctuations and a non-Curie behavior of the susceptibility but not show any T-dependence in the occupation number. We now added a comment in the corresponding section highlighting this difference. To include the additional figure in the manuscript would require the definition of the additional symmetric dimer Hamiltonian and its parameters. If the referee does not insist, we would prefer to only add the comment and keep the Figure in its original version.

3. The Clogston–Jaccarino plot should be explained.

Response: We agree with the referee that the Clogston-Jaccarino plot was not sufficiently explained in the previous version. We now added a paragraph providing more details.