March 3, 2025

Response to Referee 2

The authors address the physics of the three-band Emery model within the single-site DMFT approximation. The calculations are performed for a set of parameters, which has been recently suggested as material realistic for the cuprate superconductors. As the authors state themselves, single-site DMFT comes with limitations, foremost the failure of momentum resolving spectral functions crucially required to unravel pseudogap physics. However, this work can lay a ground on which other more advanced techniques can be rooted and should be seen as a first step towards more elaborate studies.

Within the limitations of the single-site DMFT approximation, the calculations appear to be competently carried out, and the results are presented concisely. I would nevertheless suggest several improvements to the readability, as in the current form, the manuscript only seems accessible to people at the close intersection between the DMFT community and the cuprate community.

Requested Changes

1. In Fig. 1, the color code of the band structure is referred to as "orbital character". As far as I can see, no definition in the text is provided and should be added.

   Response: We added the definition of the color code (obtained by projecting the k-dependent eigenvectors on d- and p- subspaces) in the revised version of the manuscript.

2. The authors repeatetly mention the Zhang-Rice singlet state without an explanation. The readability of the manuscript can be improved by incorporating a concise explanation of the Zhang-Rice singlet. Moreover, in Fig. 2 it should be explained why the zero energy peak corresponds to the Zhang Rice singlet. This is currently not explained well in the manuscript.

   Response: We now introduce the notion of the Zhang-Rice singlet more comprehensively and provide an extended explanation, why the zero energy peak in the spectra shown in Fig. 2 are typically interpreted as arising from this paradigmatic singlet.

3. The DMFT method is explained only very briefly in section 2. This should be expanded and a discussion of strengths and limitations should be included.

   Response: We now emphasize the strengths and weaknesses of DMFT more explicitly in the revised manuscript.

4. The shown spectral functions show rather fine features, which is remarkable as they apparently have been obtained from analytical continuation. The manuscript should explain in further detail, to which accuracy the Matsubara Greens functions are calculated and how this leads to such precise predictions on the real-frequency Greens functions.

   Response: We thank the referee for pointing out that some of the technical details were not presented sufficiently. The high resolution of the spectra on the real axis originates from the fact that we analytically continue the self-energy and not the Green function. Besides the high

resolution of the spectra, this has also the advantage that we can estimate an error-bar for the analytical continuation. We now improved the clarity of the corresponding explanation in the second to last paragraph in section 2.

5. In general, all energies are reported in electronvolt. However, to broaden the scope for other computational studies it would not hurt to also include dimensionless units, e.g. in units of some hopping in the three band model.

   Response: In principle we agree with the referee's comment that it is useful to provide dimensionless parameters. However, in multi-band Hubbard models with various hopping and interaction parameters the choice for such a unit is arbitrary as also the referee remarks in their comment. Indeed, in early stages of this work we provided all parameters in units of t_{pp} following Ref. 35 (Kowalski et al. 2021) but quickly found that this convention was rather counterproductive and led to frequent confusions especially for the comparison to experimental data (which is reported in eV and Kelvin).

   As the main conclusions of our work rely on such comparison we prefer to avoid additional units without a very specific purpose.

6. In Fig 3., the authors mention that the self-energy shows Fermi liquid behavior. The authors should specify explicitly what is meant by this and how this can be seen.

   Response: We now state more clearly that the linear real part $\mathrm{Re}[\Sigma(\omega)] \propto \omega$ and an imaginary part $\mathrm{Im}[\Sigma(\omega)] \propto \omega^2$ indicate the existance of Fermi liquid quasiparticles at low energies around $\omega \approx 0$.

7. Similarly, the authors repeatedly mention non-Curie like behavior of the magnetic susceptibility. This should be made more specific, e.g. by saying that no divergence but a maximum is observed.

   Response: We added remarks in the relevant sections of the revised manuscript.

8. The authors show a Clogston-Jaccarino plot but do not explain what this means. This plot should not be considered widespread knowledge and a short explanation would be helpful.

   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.

9. In the conclusion, the authors mention that a single band Hubbard model seems to give precise predictions for the nickelates. This statement should be weakened, as much of the community seems to agree that multi-orbital effects in the nickelates are of crucial importance.

   Response: The referee is correct in pointing out that the multi-orbital character is still subject to a controversial debate. We revised the corresponding comment in our conclusions accordingly.

I consider the present manuscript a valuable contribution to the literature and am in favor of publication. However, I am sceptical about whether the paper meets the bar of being among the top 20 percent of PRB publications required for SciPost Physics. It is unclear which of the

findings will survive a treatment with more accurate approximations beyond single-site DMFT. Even if there is better agreement with cuprates than in the single band case, it is not excluded that this is a coincidence, even though it might be an excellent hint already. I would consider a study using cluster DMFT revealing the pseudogap behavior to meet this bar, but a single-site DMFT calcution might just be too crude to induce confidence the the observed behavior is a trustworthy feature of the genuine two-dimensional Emery model. I would, therefore, rather suggest publishing the manuscript in the SciPost Core series, upon my requested changes are implemented.

Response: We thank the Referee for the comments and their judgment that our manuscript is a *"[...] valuable contribution to the literature [...]"* and their general support for publication. The referee's biggest concern lies in the shortcomings of DMFT and that we did not sufficiently exclude qualitative differences to results of more sophisticated methods like cluster DMFT.

We have now carried out the requested additional cluster DMFT calculations which demonstrate that nearest neighbor Cu-Cu correlations do not alter the temperature or doping trend we previously found.

The new comparison to CDMFT results indicate that the Cu-O correlation and the formation of Cu-O singlet fluctuations (which is included in the Emery model even when treated with single site DMFT) are key to understand the experimentally observed behavior.

The additional CDMFT results significantly strengthen our conclusions and we are indeed thankful to the referee for requesting them to *"meet the bar"* for publication in Scipost Physics.