Reply to Referee 3 considering the manuscript
"**Mott transition and pseudogap of the square-lattice Hubbard model: results from center-focused cellular dynamical mean-field theory**" ,
submitted to SciPost on 27 October 2023.

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1 General remarks

We thank all three Reviewers for their thorough reading of our manuscript and for very useful comments. Given the positive remarks of the Reviewers and the addressing of all their comments and remarks in the new version of our manuscript and the reply, we feel that our paper is now ready for publication in SciPost Physics. For clarity, figures in this reply will be labelled and referred to as Fig.Rep. which contrasts the labelling as Fig. in the manuscript. The specific remarks and requests of the referees are quoted in turqoise, followed by the respective answer.

2 Answer to the Report of Reviewer 3

First we would like to thank Reviewer 3 very much for her/his thorough reading and the valuable comments, allowing us to improve on our manuscript. We further thank Reviewer 3 for her/his appreciation of our work. We are addressing her/his remarks in the following, one-by-one:

1. **Referee:** I would suggest to detail the number of CPU hours used in order to obtained the overall results.

   Answer: We did not keep track over the overall computation cost. However, we can give details on the cost of one CDMFT data point in the more expensive parameter regime: For the data-point at $T = 0.05t$, $U = 5t$, $t' = -0.25t$, $n = 0.85$, the 4×4-CDMFT cycle, started from the converged result of $n = 0.875$ and used approximately $300'000$ core hours throughout 20 DMFT loops until convergence was reached. Here, the average perturbation order in U necessary to yield a usable sign is approximately 1300. We amended a statement to the paper in the methods section accordingly.

2. **Referee:** In order to determined Tneel is not possible to compute a stager magnetization within the cluster as order parameter? Would it lead to the same critical temperature?

   Answer: We thank the Reviewer for this question. As stated in the manuscript, we obtained the antiferromagnetic transition temperature from the fit of the physical spin susceptibility $\chi^{-1}(T)$ as e.g. in [1]. In our experience, this delivers the most precise approximation coming from the paramagnetic phase. In the alternative approach of checking for a finite magnetization it is often difficult to converge the respective impurity model very close to the (second-order) phase transition due to the divergence of the magnetic correlation length there.

3. **Referee:** I would suggest a very recent work to the authors for this half-filled analysis: Local and nonlocal electronic correlations at the metal-insulator transition in the Hubbard model in two dimensions, Maria Chatzieleftheriou, Silke Biermann, Evgeny A Stepanov

   Answer: We thank the Referee for this interesting reference. The manuscript has been adapted accordingly and the citation has been made in Sec. 3.1.

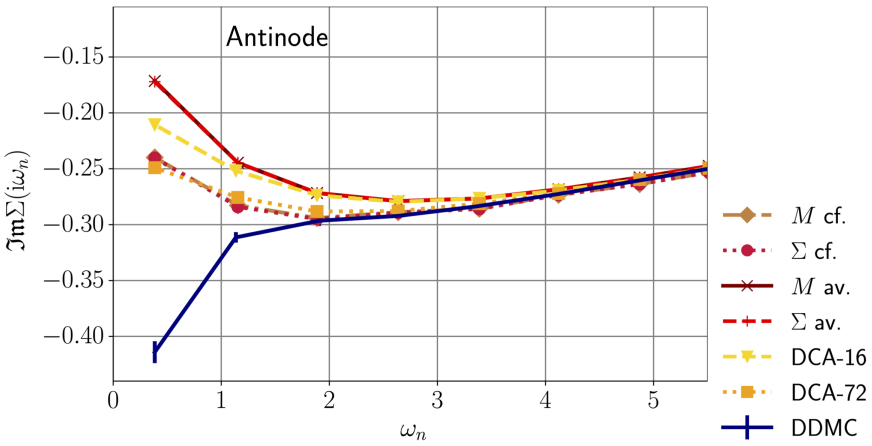

Fig.Rep. 1: Comparison of the center-focused periodization (cf.) scheme and the full Fourier transform (av.) from the Self-energy (Σ) and the cumulant (M) of the 4×4 CDMFT at the anti-node to 16- and 72 site DCA calculations and to the exact DDMC. All but the CDMFT data were taken from [2]. Plot reproduced from [3].

4. **Referee:** The periodization procedure chosen should be compared with the exact result of the Coarse grained Fourier transform within the cluster. I also wonder in respect to the methodology, if the choice of the site, where the analysis is performed, is equivalent to other choices of site within the centrals one. Would be worth to create a local self-energy of just central sites? The Self-energy are presented always for the first Matsubara frequencies but what is their behavior before imposing the cut-off at high frequencies?

   Answer: We thank the Reviewer for this important point and to answer it satisfactorily we continue by splitting the question into three parts (A,B,C):

   A On the question of the convergence of the periodization scheme: The full Fourier transform, averaging over the entire cluster yields a pseudogap only at higher interactions or lower temperatures, placing the solution of the Hubbard model further away from the thermodynamic limit. This is supported by Fig.Rep. 1, comparing the self-energy of the center-focused (cf) scheme to the one of the averaged Fourier transform (av) and to Dynamical Cluster Approximation (DCA) and Determinant Diagrammatic Monte-Carlo (DDMC) [2] at $U = 3t$, $T = 0.12t$ in the particle-hole symmetric case. In this intermediate coupling regime, both cumulant and self-energy periodization yield the same result, although the center focused (cf) periodization is much closer to the 72-site DCA calculation at the antinode, than the standard Fourier transform (av). The center focused scheme from the 4×4 CDMFT is still underestimating the self-energy considerable compared to the thermodynamic limit from DDMC in this regime of the phase diagram. The convergence of the center-focused periodization scheme with cluster size towards the thermodynamic limit was extensively discussed by Klett et al. [4].

   B On the question of the difference between center sites: The choice of the on-site component out of the different center sites does not play a role as we exploited the clusters symmetries to enhance the Monte-Carlo statistics. For an ergodic Monte-Carlo process, equivalent sites should not yield different results in the limit of an infinite number of samples.

   C On the question of the number of Matsubara frequencies: The Matsubara quantities considered in the computation were always converged with respect to the number of Matsubara frequencies used down Monte-Carlo noise (750 frequencies in each direction). In the manuscript, we analyze the consequences of the real space self-energies to the k-dependent scattering rate via the self-energy periodization, thus focusing on the low-frequency behaviour throughout the plots, indicating the quasiparticle properties. Showing the full self-energy in the overview plots of the manuscript Fig. 2-7 would have led to an unreadable low-frequency behaviour due to a lack of space. As an example, we appended the real space cluster self-energies for different fillings in the U=5t, $T = 0.05t$, $t' = -0.25t$ case, see Fig.Rep. 2, for comparison to Fig. 6 of the manuscript.

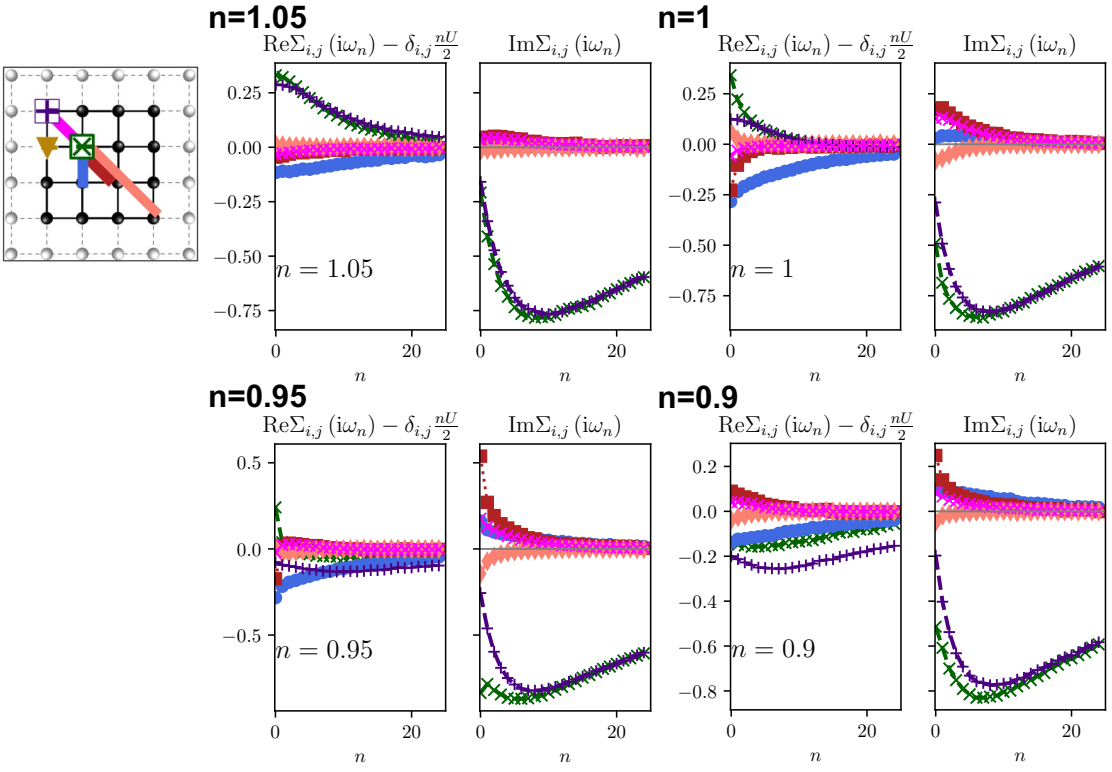

Fig.Rep. 2: Self-energies with an extended Matsubara axis window to compare to Fig. 6 in the manuscript at $U = 5t, T = 0.05t$, $t' = -0.25t$, for various fillings and different real space distances.

5. **Referee:** In Fig. 2 and then in the text there are a series of abbreviation not introduced in the extended form like nn nearest neighbor and so on.

   Answer: The abbreviations for nearest-neighbour (nn) and second-nearest-neighbour (2nn) were introduced at the beginning of Sec. 2 of the manuscript. For clarity and enhancing the readability of our manuscript we now also define 2nn in the beginning of Sec. 5.

6. **Referee:** what kind of procedure MaxEnt was used in order to obtained real frequencies data?

   Answer: A cost function between the imaginary time Green function and the spectral function was minimized. The details of the algorithm provided by the TRIQS [5] collaboration are given by [6], which is cited in the manuscript. The used cost-function exploits simplifications proposed by [7] and is preimplemented in the TRIQS algorithm. These details have been amended to the manuscript. The procedure of continuing the imaginary time Green function is referred to by the TRIQS documentation[1] as "Tau-MaxEnt" with a "Bryan"-type cost function.

7. **Referee:** Fig. 10 is somehow confusing. I would expect that by summing up all contributions of the deviation we should obtain 0, but this is not always the case. How is the occupation of the system computed? Couldn't be computed as an average over the occupation per-site?

   Answer: We thank the reviewer on her/his remark on Fig. 10 of the manuscript. We want to clarify that the numbers in the plot are rounded to the first digit behind the decimal point, i.e. 0.1%, for readability, while the total filling of the cluster as the average over the sites takes into account the non-rounded filling per site. The caption of the plot has been amended accordingly.

8. **Referee:** The use of reference 32 as example of the study of SC phase should be amended given that the results presented problem of Ergodicity (Sémon, P., G. Sordi, and A-MS Tremblay. "Ergodicity of the hybridization-expansion Monte Carlo algorithm for broken-symmetry states." Physical Review B 89.16 (2014): 165113)

   Answer: The references have been updated accordingly.

[1] https://triqs.github.io/maxent/latest/guide/tau_maxent.html

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