Reply to Reviewer 1, Mr. Downey, 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.

Michael Meixner[1], Henri Menke[1], Marcel Klett[1], Sarah Heinzelmann[2], Sabine Andergassen[3], Philipp Hansmann[4], and Thomas Schäfer[1⋆]

1 Max Planck Institute for Solid State Research, Stuttgart, Germany
2 Institute for Theoretical Physics and Center for Quantum Science, University of Tübingen, Tübingen, Germany
3 Institute for Solid State Physics and Institute of Information Systems Engineering, Vienna University of Technology, Vienna, Austria
4 Department of Physics, Friedrich-Alexander-University Erlangen-Nürnberg, Erlangen, Germany
⋆ t.schaefer@fkf.mpg.de

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 1, Mr. P-O. Downey

We thank Mr. Downey very much for his thorough reading of the manuscript, the valuable comments which helped us to improve our manuscript, and for strongly recommending the publication of our article in SciPost Physics. We will address his "Report" points in the following one-by-one, labelled with the respective number.

1. **Referee:** Page 3 line 11, a typo was probably introduced. I believe it should be "serves" instead of "servers".
   Answer: The typo has been corrected.

2. **Referee:** Maybe these are is just a details, but maybe the $T_{\text{Néel}}^{4\times4}$ and $T_{\text{Néel}}^{6\times6}$ should be written with $\times$ instead of x.
   Answer: The labels have been corrected accordingly.

3. **Referee:** Maybe the color of $T_{\text{Néel}}^{6\times6}$ should be the same as the 6×6 Widom line.
   Answer: The color scheme has been changed accordingly.

4. **Referee:** In page 9, the authors discuss the pseudogap at half filling, but Fig. 4 a) seems to suggest that there is a strong folding of the Fermi surface. In my opinion, such behavior is associated to an AFM phase and may not account for a pseudogap phase, unless the "Fermi surface" of those pockets near the border of the Brillouin zone are shown to have no coherent quasi-particles. Can the author confirm this and mention it in the text? (I don't think this needs a new figure, but I believe this needs to be mentioned)
   Answer: We thank Mr. Downey for pointing our his observations. First, we want to state that a paramagnetic solution of the system is enforced, so a folding of the Fermi surface hints towards strong antiferromagnetic fluctuations in a paramagnetic phase. Second, we point out, that this question depends fundamentally on the definition of the Fermi surface, for which we have chosen the solution of the quasiparticle equation, which does not show a folding at the antiferromagnetic zone boundary. However, the quasiparticle spectral weight obtained from the Matsubara data do, resulting in a different location of the antinode, see Fig.Rep. 1 a), red vs. orange point. Repeating the analysis of Fig. 4 of the manuscript gives the same qualitative result for both definitions of the antinode, which

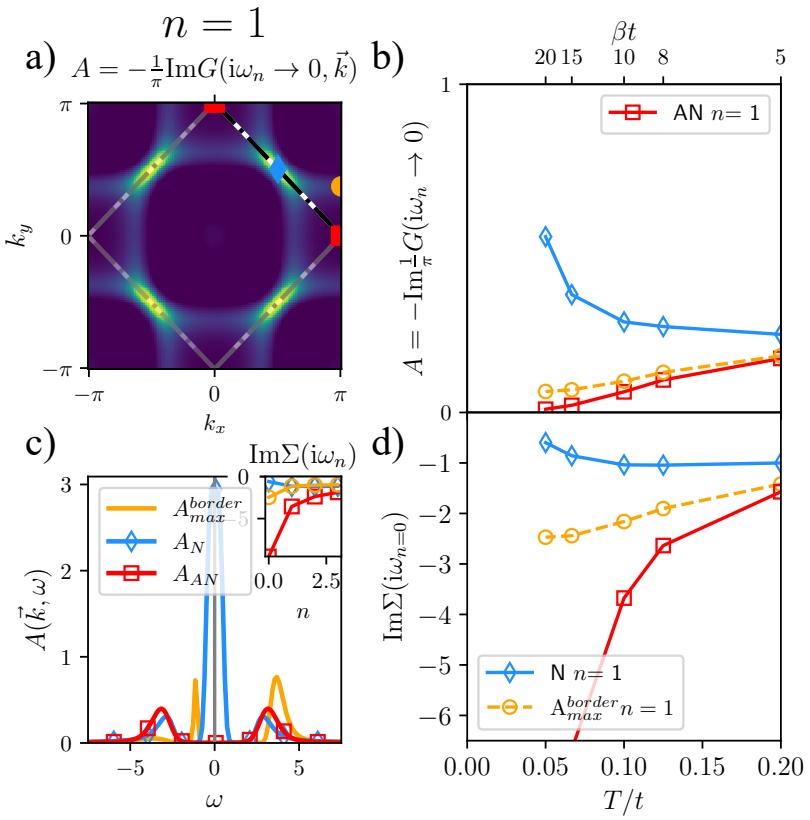

Fig.Rep. 1: a) Fermi surfaces and spectral weights (color coded), extrapolated from the Matsubara axis for $U = 5t$, $t' = 0t$, and $T = 0.05t$ obtained from the $N_c = 4 \times 4$ cluster and center-focused periodization, for the half-filled case. White solid lines indicate the non-interacting Fermi surfaces, black dotted-dashed lines the respective interacting ones. b) The spectral weight at antinode and node as a function of the temperature and filling. c) Analytically continued spectral function for the antinode (red), node (blue) and the maximum of the spectral weight at the edge of the Brillouin zone (orange). The insets show the imaginary part of the self-energies as a function of the Matsubara index for the antinode and node. d) Imaginary part of the self-energy at the first Matsubara frequency as a function of temperature. Red squares denote the antinode, blue diamonds the node throughout the figure.

allow to deduce a pseudogap as a suppressed spectral weight when reducing the systems temperature for either definition of the Fermi surface.

5. **Referee:** Perhaps I missed it in the text, but for Fig 4 a) and b), how do the authors make the extrapolation of the imaginary part of the Green's function near $\omega = 0$? I guess it is a polynomial fit, but what is the order?

   Answer: In the last paragraph of section 2.3 (Methods), it is indicated that all extrapolations to $i\omega_n \to 0^+$ are executed as a second order polynomial fit on the first three Matsubara frequencies.

6. **Referee:** Both Fig. 7 and 9 are consistent, relating to the inexistence of a pseudogap at half filling. What I find quite surprising is that this does not match what is usually seen in the litterature. Particularly, - Ref.[75] shows that the pseudogap on the electron doped side should survive up to 4% of doping at $U = 7.0$ and $t' = -0.25$ (Figure 2, $t' = 0.25$, using pte-hole transformation).
   - Ref. PRB 71, 134527 (2005) shows that the two and one band Hubbard model (Fig. 4 and 14) have an electron doped pseudogap
   - Ref. [24] shows the existence of T^* on the triangular lattice at half filling.
   - Ref. PRB 89, 245130 (2014) shows that the anisotropic triangular lattice does have a pseudogap at half filling.
   The fact that you do not find it is, in my opinion, probably because U is too small to see it. This may

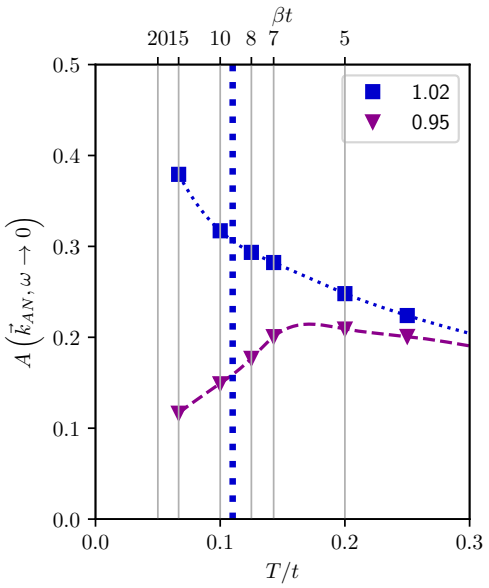

Fig.Rep. 2: Antinodal spectral weight for filling $n = 1.02$ in comparison to $n = 0.95$, for the case of $U = 5t$, $t' = -0.25t$ of the 4×4 CDMFT. The blue-dotted vertical line gives the change of topology of the Fermi-surface from hole like at high temperatures to electron like at low temperatures in the case of $n = 1.02$.

seem unrelevant to the initial goal of the article, but I believe that a small comment on that is necessary (probably at the end of Sec. 5.4). Many believe that the electron doped pseudogap only exists in the low-interaction regime, and I wouldn't want people to misinterprete your figures, concluding that there might be no electron-doped pseudogap in the strong coupling regime.

Answer: Remark 6 of Mr. Downey considers a pseudogap in the case of $t' = -0.25t$ at half filling and in the electron doped case. Indeed for the half-filled case, we were not able to find a pseudogap. In the slightly electron doped case, where numerous studies report a pseudogap, typically at $U = 7t$, we computed a scan of the spectral weight down to $T = 0.0666t$ and $t' = -0.25t$ for our $U = 5t$ phase diagram. As the plot Fig.Rep. 2 shows, a pseudogap in the case of $n = 1.02$ electron doping is not apparent and for $T < 0.11t$, the Fermi-surface changes its topology towards electron-like. This contrasts the hole-doped case of $n = 0.95$, where no Fermi-surface renormalization is apparent and a pseudogap opens for lower temperatures. We agree with Mr. Downey that this hints either towards a too small value of the interaction strengths or to a too small cluster to capture long-range correlations properly. We amended a comment to section 5.4 of the manuscript, giving the results of the aforegoing analysis and findings from respective literature.

7. **Referee:** On Fig. 10, the authors should mention that the values are given in "%" since I was confused during my first reading.

   Answer: The caption of Fig. 10 in the manuscript has been amended accordingly.

8. **Referee:** Maybe I missed the explaination in the text, but why can you conclude that there is charge density wave while it is shown earlier that central sites converge faster to the infinite-size cluster MIT solution? Pseudogap solutions are usually considered as having increased effects from correlations, this might be the reason why the differentiation is higher in the pseudogap regime than in the Fermi liquid regime in Fig. 10. I think that the authors give a great explaination, but should mention the above interpretation, or give a small explaination on why faster convergence on central sites does not impact this.

   Answer: We agree with Mr. Downey in that we cannot finally conclude the occurrence of charge density waves as we indeed can not be sure, that finite-size effects do not cause the given observation. This is why we only report a remarkable coincidence of strong charge modulations/"charge (density) inhomogeneities" inside the cluster, congruent to the regime, where periodized quantities show a pseudogap. Hence the conclusion: "Our findings hint towards charge modulations inside the

pseudogap regime, however, further studies have to clarify the impact of finite-size effects (by means of larger clusters), as well as the exact nature of putative crossover/transitions (by means of two-particle susceptibilities)." It is then remarkable, that these inhomogeneities do not occur at e.g. half filling, where at least intermediate range fluctuations are expected.