

Report of Referee 1

Report

In this manuscript, the authors present a revised formulation of the multi-orbital Two-Particle-Self-Consistent (TPSC) method, addressing inconsistencies in a previous attempt. They compare the numerical results of the new formulation with those from the original approach and other many-body methods, including DMFT, ED, and D-TRILEX.

While the manuscript may warrant publication in some form, there are several open issues that, in my opinion, need to be addressed before I can recommend it for publication.

We thank the Referee for their comments and hope that in the resubmitted manuscript, we have properly taken into account the comments from both Referees, so that our manuscript is now suitable for publication.

Following the Editor advice, I have revised the v2 version that can be found on this link <https://arxiv.org/abs/2410.00962>.

1. The authors propose two different formulations of the multi-orbital TPSC method, referred to as TPSC3 and TPSC5. I am curious why this distinction arises. If one starts with the assumption that the two-particle Green's function is constructed as its disconnected part multiplied by a time-independent constant—chosen to reproduce the exact same time and position average—shouldn't this lead exclusively to TPSC5? If this is not the case, could the authors clarify the source of this ambiguity? Additionally, a diagrammatic representation of the two formulations in terms of vertices could be helpful for less-expert readers to better visualize and distinguish the different approaches.

The distinction arises because the sum over s_4 can be left inside or pulled out of the Ansatz. Due to the underlying symmetry of the bare system, both are valid choices and, in principle, should lead to consistent results as long as the TPSC (and underlying Hartree-Fock) approach is a valid Ansatz. We added a sentence to emphasize more strongly where this ambiguity comes from. Furthermore, we added an appendix where we repeated the derivation of the Ansatz equations starting from a Hubbard-Kanamori interaction. In this case, we also see this ambiguity and we point out how the variants from the main text connect to the ones in the Appendix. Starting the derivation directly from the Luttinger-Ward functional is not possible since TPSC is technically not a conserving approximation. Concerning the second question of the referee regarding an additional diagrammatic representation of the Ansatz - TPSC is very rarely presented in terms of diagrams, since it is not really a diagrammatic technique, the only diagrammatic representation is in Vilk et al. 1997. Notably, the diagrams would be identical to the ones drawn there, as internal summations are never made explicit in such diagrams. We added a comment referring to the diagrammatic representation in the main text.

2. Another point of concern is that the authors compare the TPSC results on the square lattice with methods that are not exact in two dimensions. Could the authors elaborate on the specific limitations of DMFT and D-TRILEX in capturing physics in two-dimensional systems? Additionally, could quantum corrections in two dimensions further reduce the double occupancy values? Providing clarification on these aspects would strengthen the context of the comparisons and the interpretation of the results.

While DMFT and D-Trilex are in general not exact, they pose suitable benchmarks for our purpose, as pointed out in a recent comparative work, see Phys. Rev. X 11, 011058. In essence in the limit we are considering - relatively large temperatures and small interactions - the double occupation should in principle be relatively accurately described by DMFT as in this limit it is expected to be more or less local. With D-Trilex we get obtain an estimate of corrections due to nonlocal correlations.

3. An interesting point raised by the authors concerns the limitations of the theory in the half-filled SU(4)-symmetric case at $J=0$ and with zero inter-orbital hopping. This is a peculiar case where the TPSC formulation clearly breaks down, and the authors acknowledge and discuss this, which is an important critical observation. However, this breakdown occurs in a very specific limit. I believe that for the SU(4) case at different integer fillings (i.e., $n=1,3$),

variations in the chemical potential relative to the half-filled case could lead to differences from the single-band model. How might these differences affect the comparison between single-orbital and multi-orbital TPSC?

In our understanding, the SU(4) point does not indicate a breakdown of TPSC but rather a breakdown of Hartree-Fock, which TPSC is built upon. We rewrote the whole discussion trying to emphasize more clearly what is the cause and effect of the observed breakdown. Additionally we discuss now more clearly the implications of the "wrong" thermal expectation values predicted by Hartree-Fock. Importantly, this equivalence is not changed by doping. Upon doping all that changes is the numbers in the denominator and numerator of the Ansatz but the structure of the equations stays the same. I.e. the mapping is independent of the doping (and technically also of the number of orbitals). What does change it is adding either a Hund's coupling or kinetic couplings between the orbitals.

4. One of the strengths of TPSC is its ability to compute a non-local and frequency-dependent self-energy with reasonable computational cost. However, the authors do not discuss how the new formulations might alter this quantity compared to the previous approach. I believe the authors should address this by calculating the self-energy numerically and comparing it with other many-body methods capable of evaluating this quantity such as DMFT and D-TRILEX.

We thank the referee for this comment. We performed self-energy calculations and added a comparison of our results with both DMFT and D-TRILEX.

5. I am uncertain whether comparing TPSC against ED provides meaningful quantitative insights for its potential applications. TPSC is intended for systems in the thermodynamic limit within the weak-to-intermediate coupling regime. A dimerized state may emerge in one-dimensional systems or when interaction strengths exceed the range where TPSC is effective. Additionally, a two-site model lacks a bulk structure, meaning there is no distinction between open-boundary (OBC) and periodic-boundary conditions (PBC). Since TPSC is typically applied to models with PBC, using a cluster (e.g. four site with PBC in 2D) that respects these conditions might offer a more appropriate basis for quantitative comparison.

This point strongly relates to point 3 and we admit that indeed our formulation was misleading. This section was included to strengthen our findings from the analytical discussion and is essentially a benchmark of the underlying Hartree-Fock decomposition, since indeed TPSC does not do much in this limit. We moved this section to the Appendix and reworded it to make the central points more clear.

Here there are some minor aspects that the authors could address for improving the presentation of their paper. Requested changes:

- i Why does Figure 2 appear before Figure 3, despite the first reference to Figure 2 occurring after the first reference to Figure 3 in the text?

We thank the referee for catching this misplacement. We resolved it by moving Figure 2 to the appendix.

- ii The first three panels on the left in Figure 3 depict the same quantities. I suggest displaying only one panel and noting in the caption that the three averages should be identical.

The leftmost three panels do depict three different quantities which, due to symmetry, do have the same value. We decided to keep all three to emphasize that TPSC does get this right.

- iii In the legend of figure 4 Ref. 88 is indicated. Did the authors mean Ref.90?

The referee is correct, the reference we are referring to is Ref. 90. We thank the referee for catching this mistake.

Recommendation

Ask for major revision