Report of Referee 2

Strengths

a. This paper shows how to solve a multi-orbital Hubbard system with SU(2) symmetry with TPSC. This is a great addition to the domain as TPSC has been known to show physical features unaccessible to Dynamical mean-field calculations or Monte-Carlo ones.

b. The derivations are thorough and well explained, and the author added many details in Appendices, which are all really pertinent.

c. The analysis of the limits of the Hartree-Fock decoupling is really interesting and gives insights to the limitations of TPSC in its pure form.

d. The method is benchmarked against a previous formulation of multi-orbital TPSC, DMFT and D-TRILEX

We thank the Referee for this kind summary of our work.

Weaknesses

a. Some of the claims still need further explanation and/or references.

b. There are still some mathematical errors and/or typos with small inconsistencies, but it is almost all resolved from the first submission.

Report

I have followed the redprint for my comments. It was discussed with André-Marie Tremblay. The two-particle self-consistent approach (TPSC) is an appealing method to study strongly correlated systems. It satisfies many exact results and even though multi-orbital formulations were already done before, this generalization in the SU(2) symmetry which is presented in this paper is non trivial and will be a great addition to the field. Unfortunately again, in the present form, this paper cannot be published. It needs small corrections of mathematical issues. Furthermore, there is a section in which the discussion needs either more results shown, a physical explanation or some references to back up some statements.

After the authors respond to the constructive criticism below and after further review by me or some other referee, I hope publication can be recommended.

Requested changes:

1. After the Eq. (16), the following definition is shown : $n^{s_1,s_2}_{o_1,o_2} = c^\dagger_{o_2,s_2}(\tau,\boldsymbol{r})c_{o_1,s_1}(\tau,\boldsymbol{r})$. First of all, I think the previous introduced notation should be kept here $\boldsymbol{\tau} = (\tau,\boldsymbol{r})$, for consistency. Second, shouldn't there also be a $\boldsymbol{\tau}$ dependence to $n^{s_1,s_2}_{o_1,o_2}$? Like such : $n^{s_1,s_2}_{o_1,o_2}c^\dagger_{o_2,s_2}(\boldsymbol{\tau})c_{o_1,s_1}(\boldsymbol{\tau})$?

We thank the referee for pointing this out. We made sure that we used $\boldsymbol{\tau}$ and added a sentence to explain that due to translational invariance n has no explicit $\boldsymbol{\tau}$ dependence.

2. For equation 8, but also for all of the other equations where the sum are redundant. I have to stress that equations written as is, with two sums over one index, is not mathematically valid: at least not for the equation that is written. There are many ways to keep the equation mathematically valid and explicitly show the sum: either to remove the prime over the indices that are linked with the summation operator. eg. $\sum_{s_4} c_{s_4}c_{s_1}$. To make an even greater distinction, one could use a different notation for the explicitly summed indices: e.g. $\sum_\alpha c_\alpha c_\alpha$.

We understand that our notation could lead to confusion with some readers. Therefore, we removed the redundant sums sticking to our "primed variables are summed over" notation.

3. In the same vein as the previous point, the cases of sums shown explicitly to take into account excluded orbitals, e.g. eq. (47), the $1-\delta$ could be used: keeping the indices primed and adding $1-\delta$ would mean exactly what is written in the text. e.g. $1-\delta_{o_1,o_2}c_{o_1}$.

We thank the referee for their suggestion. We removed the redundancy by removing the primeing of the variables as this is closer to the standard literature notation of the Hubbard-Kanamori Hamiltonian.

4. In Section 3.2, there is a discussion about how the approximation of local and static vertices break down as one lowers temperature. Why? First of all, the results shown in the paper are almost all at the same temperature , which is mostly a high temperature. There are no results comparing to DMFT vertices as the temperature goes down. In the papers mentioned, I have not seen any mention of locality of vertices breaking down. I want to stress here that I am not fully against that possibility, but it seems to me that this is a claim that needs backup or a physical explanation which I have not found here. Secondly, single-orbital TPSC does not fail at low temperature, except in the renormalized classical regime. And even in the renormalized classical regime with static and local vertices for doubly self-consistent TPSC, there was great correspondance with benchmarks. [Vilk, Y. M., et al. PRB 110, no. 12 (2024): 125154. https://doi.org/10.1103/PhysRevB.110.125154.]

We thank the referee for pointing out that we did not sufficiently explain this reasoning. The claim indeed is not sufficiently backed up as it is now. The arguments for this statement consists of multiple parts - First, we know from DMFT calculations of the local irreducible vertex that its frequency dependence is becoming more pronounced at either lower temperatures or stronger interactions, see e.g. [Del Re, L. and Rohringer, G., PRB 104, 235128 (2021)]. Secondly, the lowest order correction of the fully irreducible vertex - the envelope diagram - was calculated within algorithmic Matsubara integration and at low temperatures becomes more and more confined to the Fermi-surface [Taheridehkordi, A. et al., PRB 99, 035120 (2019)]. Both these arguments agree with an RG analysis in which it was shown that in the low-energy limit the two-particle vertex is RG marginal only at the Fermi-level and zero external frequencies [Metzner, W. et al., RMP 84, 299 (2012)] (arguably this argument holds for the full vertex and not necessarily for the irreducible vertex but the two findings above provide an identical result).

Recommendation

Ask for minor revision