Report of Referee 2

Report

I thank the authors for the first two replies of the first and second submission.

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 generalisation in the SU(2) symmetry which is presented in this paper is non trivial and will be a great addition to the field.

I think publication can be recommended only after the authors modify the small changes and answer some questions.

Requested changes:

1. (Question) In Sec 3: After eqs 48, 49 and 50, that show the values of the 3 vertices of TPSC as a function of U and J of the Kanamori model. We see that the right-hand side of eqs 49 and 50 are equal, does that also mean automatically that P=C? I would expect that this is not the case for TPSC5, right?

Yes, for a Hubbard Kanamori interaction the P and C channel are identical, but this is a feature of the initial interaction - not one of TPSC. The TPSC vertices follow from equation 11-13 for TPSC3 and 14-16 for TPSC5 and even from $P = C$ we see that due to the differing rhs. of the equations these can be renormalized to different values. This is much like U_c and U_s in single orbital TPSC.

2. In Eq 51: Shouldn't there be a sum over k and ν? Or maybe we used Einstein's notation and I missed the comment? But I also think there should be a normalisation term here?

Yes, the referee is correct. Thanks for catching this inconsistency. We should have either updated it to primed variables or write the sum explicitly. We decided to do the latter one.

3. Eq 52: One U should be U'? It is mentioned below that equation that U=U', so perhaps U' should appear in that equation. Or maybe looking at the Kanamori model, they should not be separated as such and just mentioning their properties (intra- or inter- orbital) is enough. I am just asking to make sure it is also clear for readers.

We see that this could be confusing and thank the referee for pointing it out. To make the equation more readable we introduced the U' in equation 52 to make identification of which term is which easier.

4. One suggestion, it is up for the authors, but I think readers would be more inclined to follow the discussion if the comparisons to DMFT were done before the isolated case of J=0 discussion, which shows and explains why TPSC fails at low J and not so much at higher J. (So Sec 3.2 before Sec 3.1) But I do understand in a way why it was done the way it is right now. So I leave it to the authors to decide.

We thank the referee for their suggestion. Both orders do have their pro and cons. The suggested ordering first shows numerical results, which are (somewhat) unsatisfactory and explains them afterwards. The current reasoning first gives an intuitive picture and then shows numerics supporting it. Both options of ordering the sections have the potential pit-fall that readers could cast aside the paper after reading the first section, either because the results are unsatisfactory or because they understand the pitfalls and do not care much about the numerics afterwards anymore. We think that the latter one is preferable over the first and therefore stick to the current ordering of sections.

5. After Eq 59: I think there is a typo, the sentence starts with "This we can . . . ".

The referee is correct that this might confuse a reader - We changed it to "This Hamiltonian we can . . . "

6. In the caption of the plots of Figure 3 : I think the number of the Reference was not updated, because it is not the same as in the citation of the same figure.

We thank the referee for catching this mistake.

7. Last paragraph of Sec. 3.3.2 : There is no direct reference to the figure that shows susceptibilities (Fig 6, I think) , even though there is a discussion about it. This seems to be just an oversight.

Indeed, we forgot to add the reference there. Thanks for catching it.

8. Figure 2b) : From what type of calculation do those results come from? Exact diagonalization, DMFT?

These results come from ED, we clarified this in the caption now.

9. In Section 3.2 : There is an explanation of the limitation of TPSC at low temperature coming from the Hartree-Fock decoupling, but then in Appendix E, it is said that Hartree Fock is more valid at low temperature, this looks like a contradiction. After a couple of re-reading, I have come to understand that the limitation at low temperature for TPSC is due to the importance of the non-local and non-static corrections on the vertices, but doesn't that also apply to Hartree-Fock?

First of all, we would like to thank the referee for this good questions since it lead to us critically reexamining our argumentation and we realized that it was oversimplified. The central issue we have here is that we argued in terms of a variational Hartree-Fock approach but technically we should have argued in terms of a diagrammatic Hartree-Fock. Since the two are identical at $T = 0$ *we can still somewhat understand what happens from the former one but to generalize our explanation we added a discussion of the observed behavior in terms of the self-energy we obtain from diagrammatic Hartree-Fock.*

Concerning the question of the referee - At low temperatures, excited states freeze out and so the thermal expectation value is approach then expectation value over the ground state (if it is non-degenerate). Thus, the expectation value we obtain from either variant of Hartree-Fock would become more reliable at low temperatures as long as the true ground state is well approximated by Hartree-Fock. Thus, we state that Hartree-Fock is expected to improve at lower temperatures. However, the aspect we indeed did not discuss is that Hartree-Fock becomes inadequate at low temperatures if the ground state manifold is either degenerate or not representable by Hartree-Fock. Therefore, we removed all statements about expecting an improvement of the underlying Hartree-Fock decomposition at lower temperatures.

Recommendation

Ask for minor revision