Report of Referee 1

Report

The new version of the manuscript is an improvement when compared to its previous one however I still have some doubts about one of the main aspect of the paper and therefore I am not convinced to recommend this paper for publication yet.

1. From what I understand, the authors argue that the source of ambiguity arises from the structure of the equation of motion, specifically whether the sum over the internal spin index is incorporated into the ansatz definition or not. However, in TPSC, the ansatz is typically chosen to reproduce the correct static and local limits of the two-particle Green's functions. This can be achieved by defining G(2) without directly relying on the equation of motion. Once this quantity is fixed at the level of G(2), it is then used in the equation of motion. My question is: would this ambiguity persist if one were to adopt this protocol for fixing the ansatz?

If we understand the referee correctly, they are referring to the physically motivated derivation of the equations as presented for example by A.-M.S. Tremblay in Two-Particle-Self-Consistent Approach for the Hubbard Model. For simplicity we will stick to a Hubbard-Kanamori interaction in the following discussion. The starting point for this derivation are the sum-rules and the RPA equation for the spin and charge vertex, respectively, in which the interaction is replaced by the renormalized spin/charge interaction. To close the set of equations we have to come up with an Ansatz for the renormalized interaction, which in this derivation does not arise in a unique way by enforcing the local and static limit of the two-particle Green's functions (I.e. in contrast to the single orbital case we still can write down multiple versions all leading to the same outcome). In a sense - the ambiguity in the Ansatz is a consequence of the multi-orbital structure of the vertex allowing for more than one unique non-zero spin component. Therefore, the suggested protocol does not address the ambiguity of enforcing the local and static limit.

2. I would honestly suggest the authors to move Figure 2 into the appendix.

We appreciate the suggestion of the referee and understand that this suggestion probably arises from the figure being purely on the toy model level. However, we decided against moving the figure to the appendix as it is referenced multiple time in the section it is embedded in.

3. The authors considered my advice to perform additional calculation partially. While I appreciate their effort in doing so I think that it would be informative to compare the self-energy computed using the different methods fixing two or more k-points as a function of frequency.

We added a plot where we compare the selfenergy as a function of frequency at the Γ, X and M point at a single interaction value $U = 2$.

Recommendation

Ask for major revision