Reply to Referee Report

General Remarks: *In the manuscript, the authors study the existence of unconventional superconductivity (SC) by using the ionic Hubbard model without doping. While being a band-insulator, a large staggered potential, comparable to the Hubbard interaction, closes the band-gap and the system shows a metallic state even at half-filling, as also shown in Ref. (24). Contrary to the pure Hubbard model, double occupancy is not energetically prohibited allowing for charge fluctuations. By using the Gutzwiller projection, the authors are able to derive a low-energy $t - t' - J - J'$ effective Hamiltonian, which is then solved by using the renormalized mean-field theory (RMFT) for the magnetic and superconducting gaps. The main results is shown in Fig.(1), where the authors found a superconducting state surrounded by paramagnetic metal and ferri metal states. As the system approaches the SC phase from the two sides, the increase of the electron pockets in the quasi-particle spectrum lead to pairing mechanisms at the Fermi surface. The main part of the article is well written and the results discussed extensively. The physical ideas are still important to warrant a publication. Hence, I recommend the publication of the manuscript once the authors addressed the comments below.*

Response : We thank the referee for positive assessment of our work. We are glad that the referee agrees that the physical ideas presented in this work are important. Below we answer the specific comments that the referee has made.

Comment 1: *It is not clear how spin fluctuations are treated and how they generate a sizable pairing gap in optics of the RMFT. I think that the paper would benefit from a better presentation of the RMFT in general, by reporting the gap equations and the magnetic correlators.*

Response : The spin exchange terms are treated at the same mean-field level as in regular $t - J$ model where the superconductivity for hole doped system has been studied extensively. For the model studied in our paper, the contribution to pairing terms comes not only from the nearest neighbour spin-exchange term but also from other dimer and trimer terms in the effective low energy Hamiltonian (described in Appendix A) resulting in finite pairing amplitude in the SC phase for both the pairing symmetries we have studied. The pairing gap seen in the single particle density of states is proportional to the rescaled couplings times the pairing amplitude, where couplings include all dimer and trimer terms that contribute to the pairing in the mean field decomposition. Following the referee's suggestions we have provided additional details of the gap equations and magnetic order parameters in section 3 of the manuscript. To provide

other details of the RMFT, we have added an appendix in the manuscript.

Comment2: The authors comment that their calculations estimate the superconducting critical temperature in cuprates. One should carefully consider that the absence of doping and a too large staggered potential might lead to a physically different situation when considering the critical temperatures. Also in the context of the spectral function, that is significantly different from the observed in cuprates. Indeed, as shown in Fig.(3), all the quasi-particles have the same spectral weight along the Fermi-surface.

Response : We are not claiming that we are estimating the superconducting critical temperature in *cuprates* through our calculations. Probably what has caused confusion is the fact that we used the hopping amplitude comparable to that in cuprates to come up with an estimation of T_c. We apologise for this confusion and we have rewritten the relevant sentences on page 7 of the manuscript to clearly bring out what we meant to say.

What we were trying to do was get a rough estimate of the T_c for the model we have studied. For this purpose, we need an energy scale for the hopping amplitude in our model. From our analysis $T_c \sim 0.03t$. We are only trying to say that if the hopping amplitude for the ionic-Hubbard model is comparable to that of cuprates, then the estimated T_c also comes out to be pretty large, in the same range as the T_c of cuprates.

In fact in the very beginning of the paper in the introduction we have mentioned that the model we have studied is different from those used for conventional HTSC like cuprates. Exactly as the referee pointed out, due to the strong staggered potential $\Delta \sim U$ the physics of the model we study is very different from that of the cuprates. We have clearly written in the conclusion section "A remarkable feature is that the SC phase in this model of a correlated band insulator is sandwiched between paramagnetic metallic and ferrimagnetic metallic phases (Fig. 2[e]), which makes the zero temperature phase diagram very different from that of the known unconventional superconductors like high Tc cuprates" The only similarity between the SC in our model and the cuprates might be the presence of a pseudogap phase, but we are nowhere claiming to estimate the T_c for cuprates from our study.

About the spectral functions in Fig.(3): These are low energy $A(k, w)$ color plots in the ferrimagnetic and paramagnetic metallic phases that appear on two sides of the SC phase as U/Δ is tuned. These phases don't even appear in the phase diagram of cuprates and hence as the referee has correctly pointed out, these spectral function are significantly different from those observed in cuprates. To further clarify why all the quasiparticles have the same spectral weight along the Fermi surface in the metallic phases for which $A(k, w)$ has been shown, we have added

a few lines in the section on Spectral functions about it. Basically we are showing the spectral function for the Green's function averaged over both the sublattices $[G_{AA}(k,w)+G_{BB}(k,w)]/2$ for which the quasiparticle weight is same along the entire Fermi pocket though individually if one looks at the spectral functions of $G_{AA}(k,w)$ or $G_{BB}(k,w)$ they show variation along the Fermi pockets.

Comment3: The value of t' is positive (with respect to t), while usually a negative t' is used. The difference lead to the presence of hole-pockets at $k=(\pi/2,\pi/2)$ instead of el-pockets. How would the system behave with a negative t'?

Response: We thank the referee for this comment. We wanted to make an explicit comment about it in the manuscript but somehow it got omitted. The physics of t' positive and t' negative is simply related by particle-hole transformation shown below

$$C^{\dagger}_{iA\sigma} \rightarrow -C_{iB\sigma} \tag{1}$$

$$C^{\dagger}_{iB\sigma} \rightarrow C_{iA\sigma} \tag{2}$$

Under this transformation, $n_{iA\sigma} \rightarrow 1-n_{iB\sigma}$ and $n_{iB\sigma} \rightarrow 1-n_{iA\sigma}$. The Hamiltonian of the IHM with t' maps to the one with $-t'$, that is the model in eqn (1) of the paper gets transformed to

$$H = -t \sum_{<ij>\sigma} C^{\dagger}_{iA\sigma} C_{jB\sigma} + h.c + \Delta \sum_{i\in A} n_{iA} - \Delta \sum_{i\in B} n_{iB} \tag{3}$$

$$+t' \sum_{<<ij>>} C^{\dagger}_{iA\sigma} C_{jA\sigma} + C^{\dagger}_{iB\sigma} C_{jB\sigma} + h.c. + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{4}$$

As an effect of this particle hole transformation, $m_A \rightarrow -m_B$ and vice-versa. Hence, $m_s = m_A - m_B$ remains unchanged but $m_f = m_A + m_B \rightarrow -m_f$. Also the hole and electron pocktes in the spectral function and the momentum distribution function get interchanged as pointed out by the referee. But as far as the basic physics and the phase diagram obtained is concerned it remains unchanged for $+ve$ or $-ve$ values of t'. This becomes clear from the figures shown below where we have shown the order parameters, spectral functions and momentum distribution function for $t'=-0.45$ and compared with those of $t'=0.45$. We have also added a comment about it in the manuscript in section 2.

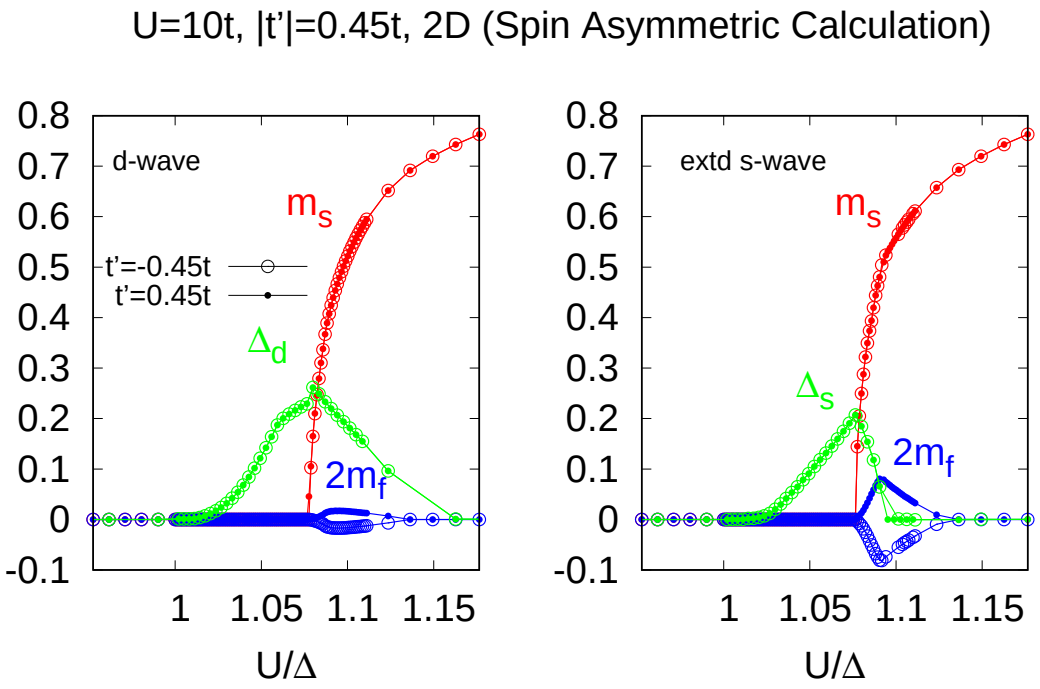

Figure 1: The pairing amplitude and magnetic order parameters for $t' = -0.45$ and $t' = 0.45$. As shown only m_f changes due to related particle hole symmetry between the model with $+ve$ and $-ve$ values of t'.

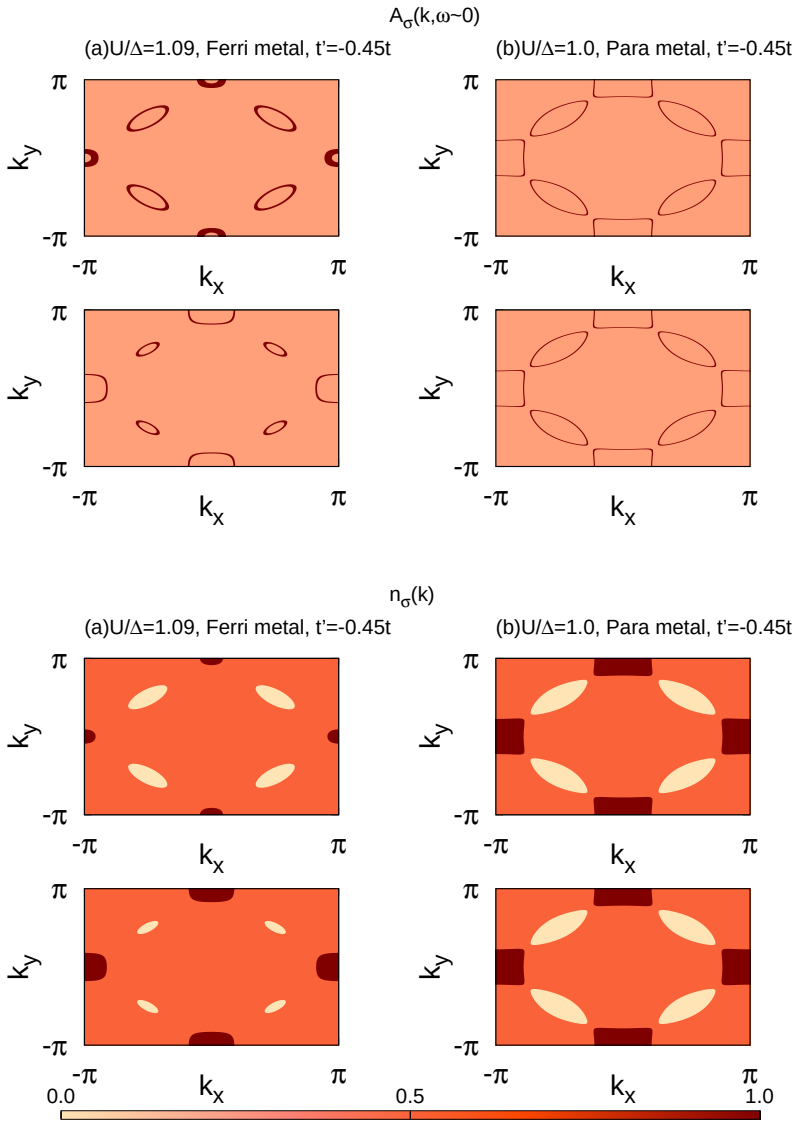

Figure 2: Top panel shows the spectral functions in the metallic phases for $t' = -0.45$. First row is for spin-up and the second row is for the spin-down component. The bottom panel shows the momentum distribution function $n_{k\sigma}$ in the metallic phases for $t' = -0.45$. Comparison of this plot with the one in the manuscript shows that the hole and electron pockets get interchanged for negative values of t'. For negative value of t' we have electron pockets around $(\pm\pi, 0)$ and symmetrically related points while we have hole pockets around $(\pm\pi/2, \pm\pi/2)$ points.