We thank the Referee for the detailed report that helped us to considerably improve our manuscript. Below please find our response (in black) to all comments, questions, or suggestions raised by the Referee (in blue).

We note that in the revised version of our manuscript, we have adopted the latex template for Scipost Physics, as suggested by the journal instructions. This implies that the numbering of the sections changed from Roman to Arabic (i.e., II.C -> 2.3 and so on). In our response, we will consistently use Arabic numbering of sections.

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The manuscript titled "Boson-fermion pairing and condensation in two-dimensional Bose-Fermi mixtures" investigates the phase diagram of a two-dimensional mixture of a Bose gas and a Fermi gas which are coupled via a strong interaction that can feature bound states even in the two-body limit. The work builds on previous analyses conducted in three dimensions which utilized the same type of diagrams. Due to the presence of condensed bosons, the fermionic and the molecular sector are hybridized into a joint excitation and thus the relevant quasiparticles are superpositions of these two sectors. To illuminate this mechanism, the authors derive analytic expressions –valid in the strong-coupling regime– which showcase the different quasiparticles at play. In the relevant regimes, their fully numerical treatment shows good overlap with their analytic expressions, and they find subtle physical differences (and also similarities) compared to the corresponding physical system in three dimensions. While, as in 3D, they find that increasing the Bose-Fermi interaction strength progressively depletes the condensate, they do not find the condensate fraction to vanish beyond a critical interaction strength (unlike in 3D). As a result, the emerging quasiparticle show some unusual features. Like in 3D, a universal behavior with respect to the ratio between bosonic and fermionic density is found for quantities like the condensate fraction.

The present manuscript is timely, and the physics covered is certainly interesting. I am not aware of previous works that have addressed this phase diagram along with the interplay of pairing and condensation in two dimensions. As mentioned in the main text, an experimental implementation of an analogous system in three dimensions was demonstrated recently and thus two-dimensional

implementations are certainly within reach (and have already been studied in the polaron limits). Insights into the qualitative physics in two dimensions along with the differences to analogous systems in three dimensions are thus welcome and provide great progress to the field.

While this manuscript is certainly worthy of publication, there are a few issues/comments/ questions I would like to see addressed before recommending publication. I provide the comments below.

We thank the Referee for the above appreciation of our work and for judging it certainly worthy of publication.

Before getting into content feedback, I would like to encourage the authors to proofread the manuscript thoroughly. While reading through the manuscript, I found several instances of unnecessarily long/complicated sentences that required several readings before I was able to understand them. I also found several sentences missing verbs or with singular/plural errors. I invite the authors to conduct another round of proofreading to facilitate readability for all readers.

We have simplified several long sentences throughout the manuscript and carefully proofread it.

While the technical analysis conducted in this manuscript is sound (though in some instances I think the presentation may be improved), my main concerns are the diagrammatics used and the physical conclusions one may draw from it. I am fully aware, that the present analysis is challenging enough as is and going beyond it, taking into account higher-order effects or higher degrees of self-consistency is no easy feat. I feel however, that this manuscript lacks transparency in its main drawback, and I would like to see this discussed more. As I am sure the authors are fully aware, in the normal phase this type of T-matrix approach has a central drawback: it treats renormalization of the molecule sector and renormalization of the fermion sector on a different footing. As a result, in the Fermi-polaron limit of $n_B=0$, $n_F>0$ in three dimensions the molecule's energy is higher than it should be, and the polaron-to-molecule transition takes place later than it does in more self-consistent approaches. Apart from that, the Ansatz gives qualitatively correct results, especially in observables that do not include the energy (such as the quasiparticle weight). In two dimensions, however, this Ansatz no longer holds a polaron-to-molecule transition, even though several state-of-the-art methods

do find one. This of course has implications also for the phase diagram and phase transitions of 2D B-F mixtures, as the present approach cannot reproduce known physics for x->0 at large g. This does not mean that at larger values of x it must produce incorrect results, but it is at least a possibility.

The authors mention this point in the conclusion, but I feel that in the interest of transparency it must be stated also in other places in the main text, especially when the diagrammatic is motivated due to its success in 3D or when results for large g and smaller values of x are discussed. It is also not clear to me how, when having a vanishing condensate fraction for x=0, this is regenerated upon going to x>0. Of course, I cannot discount the possibility that in 2D no phase transition exists, and one may rather see somewhat of a crossover, but this cannot be inferred from the analysis conducted here and I feel that the reader should be made aware of this potential shortfall BEFORE they get to the conclusion. I strongly encourage the authors to make mention of this, especially when pointing out differences between two and three dimensions, which may possibly only be due to this simple shortfall. I don't think mentioning it lessens the great value of their work.

As suggested by the Referee, we now discuss the absence of the polaron-to-molecule transition in 2D within the present T-matrix approach already in Sec 2.2, when we motivate it due to its success in three dimensions, as well as in Sec. 4.4, when pointing out differences between two and three dimensions.

See, in particular, the second paragraph of Sec. 2.2 and the last paragraph of Sec. 4.4.

In Figure 14, no correspondence between the condensate fraction and the Z factor is found. This is highly surprising to me as from a simple Chevy Ansatz one can see a close correspondence between the two. Is this difference because the chosen values of x were not small enough? If true, this is a major difference between 2D and 3D. Certainly one which has nothing to do with the absence of a polaron-molecule transition. Could the authors illuminate/investigate this further? For x->0 or at least for x=0, these two observables should be the same, so I am very surprised they are different.

In Figure 14(a) we have now added data for the condensate fraction at a smaller value of x ($x = 0.01$) that confirms the absence of the correspondence between the condensate fraction and Z in 2D. Furthermore, we have added the result for Z from the derivative of the bosonic self-energy with

respect to the frequency by using the same code used at finite x, adapted to the single-impurity limit. Our results (diamonds) fully agree with the corresponding results for Z previously obtained within the same non-self-consistent T-matrix approach for a single impurity in a Fermi sea (circles), thus showing that the discrepancy between Z and the condensate fraction cannot be ascribed to possible numerical errors. As a matter of fact, and contrary to what we argued some time ago in Ref. 91, we now believe that there is no reason why the limit for $x \to 0$ of the condensate fraction and the polaron residue Z should coincide. The first quantity is defined by the ratio between the number of condensed bosons N_0 and the total number of bosons N_B in the thermodynamic limit $(N_\mathrm{B} \to \infty, V \to \infty$, at fixed n_B and x). It is only in this limit that a condensate fraction is well defined. So, no matter how small x is, the number of bosons N_B will always scale to infinity in the thermodynamic limit, while in the polaron limit one has instead $N_\mathrm{B} = 1$. Therefore, the occupancy of the zero-momentum state for a single impurity cannot be in general related to the ratio N_0/N_B in the limit $x \to 0$. It is a matter of order of limits. In the first case (condensate fraction), one first fixes x, takes the thermodynamic limit $V \to \infty$, and finally let $x \to 0$. In the second case (polaron Z), one first fixes $N_\mathrm{B} = 1$ and then takes the limit $V \to \infty$ in such a way that $x = 1/(n_\mathrm{F}V) \to 0$. It is thus clear that in this second case, the thermodynamic limit and the limit $x \to 0$ are taken simultaneously, while in the first case the thermodynamic limit is taken first, followed by the limit $x \to 0$.

In the 3rd and 4th paragraph of Sec. 4.4 we now clarify this subtle point.

Other feedback (in no particular order):

1. While I am familiar with the diagrammatics used, I am afraid many readers might not find them easily accessible. I feel that confusion might originate from the differences between the Gamma and T vertex in Figure 1 and how these diagrams are obtained. I suggest to either a) expand on an explanation of how the diagrammatics can be obtained (possibly in an appendix), b) provide a reference where this is done, or c) conduct parts of the explanation in a two-channel language (done recently in Ref. 53), where their different roles are more clear. I am not aware of Ref 73 or Ref 88 providing a more accessible explanation. In section 2B the Gamma vertex is referred to as a T-matrix; while I am aware that for n0=0 they are the same thing, this can easily add to confusion. I suggest to

We now consistently use throughout the manuscript different wording when referring to $\Gamma(\mathbf{P}, \Omega)$ and $T(\mathbf{P}, \Omega)$, as suggested by the Referee. Specifically, we now refer to $\Gamma(\mathbf{P}, \Omega)$ as "particle-particle ladder" and to $T(\mathbf{P}, \Omega)$ as "many-body T-matrix in the condensed phase".

Concerning the point on "an explanation on how the diagrammatics is obtained", our strategy in constructing the diagrammatics is as follows. Out of all possible Feynman diagrams, we have selected a particular class of diagrams (ladder diagrams) that, since the pioneering work by Nozieres and Schmitt-Rink (Ref. 100) on the related problem of the BCS-BEC crossover in two-component Fermi gases, is well known to capture pairing (molecular) correlations in the normal phase (see also Ref. 101 for a review). It is only after the inclusion of this class of diagrams that the superfluid critical temperature recovers the Bose-Einstein condensation temperature in the strong-coupling limit of the BCS-BEC crossover. In addition, for the same contact potential we are considering, ladder diagrams also provide the leading self-energy (established many years ago in Ref. 102) in the weak-coupling limit. They thus provide a sensible scheme to describe the whole BCS-BEC crossover, even in the intermediate coupling region in which fully controlled approximations are not available. The same strategy is then adopted for the present problem, in which we are interested in setting up a theory that is able to describe the progressive formation of pairing (molecular) correlations in a Bose-Fermi mixture, when the BF interaction is varied from weak to strong.

When switching to this problem, the required modification is straightforward in the normal phase: the particle-particle ladder made of the repeated interaction of spin-up and spin-down fermions is replaced by a particle-particle ladder made of the repeated interaction of bosons with (one-component) fermions. When extending the theory to the condensed phase, one has to take into account the possibility that fermions repeatedly interact also with condensed bosons, besides non-condensed bosons. By summing all possible combinations of the repeated scattering of fermions with condensed or non-condensed bosons one obtains the many-body T-matrix in the condensed phase described by the Feynman diagram of Fig. 1. Finally, like in the corresponding problem for the

BCS-BEC crossover, when constructing the T-matrix self-energy of one species, the T-matrix needs to be closed by a propagator of the other species. For the fermionic self-energy in the condensed phase, the bosonic line might be either a condensed line or a non-condensed line. In the first case, however, the many-body T-matrix in the condensed phase $T(\mathbf{P}, \Omega)$ needs to be replaced by $\Gamma(\mathbf{P}, \Omega)$ in order for the self-energy to be irreducible (and thus avoiding a double-counting of diagrams when inserting the self-energy in the Dyson equation).

We wish, finally, to emphasize that, similarly to the corresponding theoretical approach for the BCS-BEC crossover, our choice of diagrams, besides capturing boson-fermion pairing for strong BF coupling, also reproduces the perturbative results of Ref. 104 in the opposite weak-coupling limit, as explicitly shown in Sec. 4.3. It is thus expected to provide a sensible first approximation to describe the whole evolution from weak to strong coupling.

We have now added the above comments justifying our choice of diagrams in the revised version of the manuscript. See in particular, the third and fourth paragraphs of Sec. 2.2, the paragraph just above Eq. 7, the paragraph just above Eq. 9, the paragraph just below Eq. 11, the first sentence after Eq. 55, and the last sentence of section 4.3.

2. I appreciate the analysis conducted in section 3 to illuminate the nature of the quasiparticles resulting from hybridization, however in part I find it very hard to follow due to its very technical nature and the non-trivial effects of hybridization. The analysis in 3A is easy to follow, I would possibly ask that the E+ and E- excitations are related also to the undressed states they correspond to for vanishing condensate density.

The relation between the hybridized dispersions E^+, E^- and the unhybridized ones $\tilde{\xi}_{\mathbf{P}}^{\mathrm{CF}}, \xi_{\mathbf{P}}^{\mathrm{F}}$ depends on the sign of $\tilde{\xi}_{\mathbf{P}}^{\mathrm{CF}} - \xi_{\mathbf{P}}^{\mathrm{F}}$. We have added this remark in section 3.1, in the new paragraph starting with "One sees from Eq. 29 ..." shortly after Eq. 29. The sign of $\tilde{\xi}_{\mathbf{P}}^{\mathrm{CF}} - \xi_{\mathbf{P}}^{\mathrm{F}}$, on the other hand, depends on the value of the chemical potentials $\tilde{\mu}_{\mathrm{CF}}, \mu_{\mathrm{F}}$, and on $\mathbf{P}$, in general. Since the chemical potentials are calculated later on in section 3.4, a more explicit discussion of the limiting values of E^+, E^- for vanishing hybridization is done in that section (see paragraph in sec. 3.4 starting with "Let us now analyze in detail the effect of the hybridization scale" and the paragraph following it).

In addition, this remark by the Referee, together with the remark 24 below, prompted us to clarify already in section 3.1 that $n_0 \to 0$ does not necessarily imply $\Delta_0 \to 0$. This is done at the end of the paragraph starting with "One sees from Eq. 29 ..." shortly after Eq. 29.

3. The analysis in section 3B I found very hard to follow and I wonder whether it is necessary in the place it occurs now. It is my understanding that section 3 serves to illuminate the underlying quasiparticle qualitatively, mainly to shine light on the effects of hybridization:
In section 3A the T-matrix is analyzed, and one finds that it mixes unpaired atoms with molecules. The quantum fluctuations taken into account are a self-energy renormalization of the molecule (contained within Gamma). As a result, the two excitations found within T are a result of the mixing of a non-renormalized atom with a renormalized molecule. These two excitations would also show up in the same way if one considered a corresponding fermionic Green's function (of course the distribution of quasiparticle weight between them would be different). However, the fermionic Green's function in this work is considered on different footing and mixes a renormalized molecule with a renormalized fermion, resulting in two (slightly) different excitations. I am however not sure that this different, second set of excitations, introduced in 3B and analyzed after Eq. 32 for Delta0/EF small is actually needed in this detail. Maybe the part with Delta0/EF small is better suited for an appendix? When references to the analytical expressions were made later in the text, I could only really find references to 3A and parts up to Eq. 32. The reason I bring this up, is that I found this part (after Eq. 32 until before Eq. 47) extremely challenging to follow, due to its technical nature and I am not sure which physical insights are conveyed in it. Furthermore, it had the effect that in section 3D and onwards I found it challenging to follow which analytical results were being referred to, those mainly from 3A or those from 3B.
We have implemented the suggestion by the Referee and moved the details of the expansion for small Δ_0/E_{F} to Appendix D.2. We now keep in section 3.2 only the final equations describing the fermion momentum distribution for small Δ_0 (Eqs. 41-43). We decided to keep these equations because they are referred to in sec 3.4 when discussing the fermionic momentum distribution in the strong coupling limit (see comments to Fig. 6). In addition, in this section, we have completely rewritten

the paragraphs discussing Fig. 6 (see last three paragraphs of Sec. 3.4). It should now be clear when we refer to the small Δ_0/E_F expansion.

    4. Are there cheap ways to enforce a polaron-to-molecule transition, along with the corresponding physics? For example, in the analytical results obtained in Section 3. If yes, how do the results obtained from that look like?

Actually, even before the first submission, we endeavored to find a simple way to enforce a polaron-to-molecule transition but did not succeed. We tried again, but we did not reach any definite conclusion so far.

    5. Using the same diagrammatics in 3D, in Figure 7 of Ref. 77 a peculiar bosonic distribution function was observed, which vanished identically below a certain momentum. This was due to the bosons participating in fermionic molecule formation and as a result, the bosonic distribution function showed remnants of a fermionic effect. Can something analogous be observed here in 2D?

The peculiar distribution function of former Ref. 77 (now Ref. 80) was found in the normal phase, i.e., when the molecular correlations are so strong to suppress completely the condensate. In the present 2D case, as already mentioned, even when $n_0 \rightarrow 0$ in the strong-coupling limit, the hybridization energy scale Δ_0 does not vanish in general. The presence of this hybridization essentially removes this effect. Possibly, a small remnant of this effect is visible in the data of Fig. 7 for $g = 1.2$ and $x = 0.175$ and $x = 0.5$. One may see a kind of bimodal distribution for $n_B(k)$. The feature at small k is attributed to the presence of hybridization caused by a non-zero condensate. The second feature at larger k instead resembles the one found in 3D with remnants of a fermionic effect. The same behavior occurs in the data for $g = 2$, but it is not visible in Fig. 7 due to the scale used for the y-axis. Data are however available in the data repository quoted in the revised version of the manuscript (Ref. 133).

    6. I find the used terminology of dressed/undressed dangerous. As is, "dressed" refers to the effects of hybridization (which one may see as resulting from a Green's matrix inversion in a two-channel language) and "undressed" refers to effects without hybridization. However, the undressed propagator still contains quantum fluctuations. In section 3A the adjective "bare" is used

below equation 25. However, that molecule still contains quantum fluctuations, albeit in a mean-field fashion through SigmaCF. Maybe the authors mean undressed? In any case, I feel these ambiguities can be a source of confusion for many readers and I would ask that the authors explain exactly what they mean when they use adjectives like dressed/undressed/bare.

The Referee correctly interpreted our use of "dressed" and "undressed" with respect to the effects of hybridization and we agree with the Referee that the use of "bare" below former Eqs. 21,25 was misleading. We now clarify, in the text around current Eq. 24, that $P^2/2M - \mu_{CF}$ is the dispersion of a bare molecule and that $P^2/2M - \tilde{\mu}_{CF}$ is the same dispersion renormalized by the mean-field shift Σ_{CF}^0 (we point out that we have now replaced the old name Σ_{CF} with the new one Σ_{CF}^0 in order to adopt the same convention used for the mean-field shift Σ_F^0 of the atomic assembly). In addition, after Eq. 27 we now clarify the use of "dressed" and "undressed" in relation to hybridization. Finally, we have found that in some other places in the manuscript we used the adjective "dressed" in a broader sense (i.e., not referring to hybridization but to more generic effects of interactions). In these cases, we have replaced "dressed" with "renormalized" to avoid any possible misunderstanding.

7. I believe an analytical expression for Eq. 5 was provided in Ref. 106

We thank the Referee for this remark. We missed that an analytical expression for $\Gamma(\mathbf{P}, \Omega)$ was already reported in former Ref. 106 (now Ref. 121). We note, however, that the equation of Ref. 121 is valid for the case of equal masses and frequencies on the real axis, while our expression is valid for generic masses and imaginary frequencies. Stimulated by the compactness of the expression reported in Ref. 121, we have recast our analytical expression for $\Gamma(\mathbf{P}, \Omega)$ in an analogous way. From this expression one can easily see that, for equal masses, our expression recovers the corresponding equation of Ref. 121 after the analytic continuation $i\Omega \rightarrow \omega + i0^+$ is performed. In Appendix A, we have added a comment on this correspondence.

8. Where is the condensate factor introduced? It briefly appears in the caption to Figure 1 and in the main text it starts appearing in Eq. 6, but there is no proper mention of what it actually is there.

We now explicitly mention what n_0 is the first time it is introduced (see last paragraph of Sec. 2.1).

9. In Eq. 8 the convergence factor appears but there is no mention of it.

We have added a brief comment on the convergence factor $e^{i\Omega 0^+}$ below Eq. 9.

10. In Eq. 2, it is v0 while other times it is nu0.

We thank the Referee for pointing out this inconsistency. We have fixed it.

11. I believe the renormalization/regularization in Eq.2 would benefit from a reference.

We have added two references discussing the regularization in Eq. 2 for the analogous case of a 2D Fermi gas (Refs. 95-96).

12. Is Omega a real or an imaginary frequency?

In the first version of the manuscript (after former Eq. 5, now Eq. 6), we actually already specified that we work with imaginary frequencies. However, to make it even clearer, we now report Eq. 5 for $\Gamma(\mathbf{P}, \Omega)$, where the explicit dependence on Ω is apparent. This equation (previously reported in Appendix A) should clarify this point with no ambiguities.

13. Are there things one can say about T>0?

At T > 0, long-range order is prohibited by Mermin-Wagner theorem. At finite temperature, the T=0 condensed phase will become a BKT superfluid phase with quasi-long-range order for the bosonic component. Similarly to T=0, we expect Bose-Fermi pairing to compete with the bosonic superfluid phase. A quantitative description of this competition at finite temperature would be extremely interesting, but it is clearly out of the scope of the present work. In addition, it is not clear to us how the BKT physics of the bosonic component could be effectively introduced in our diagrammatic scheme. A comment on T > 0 has been added at the end of the conclusions.

14. The authors set mB=mF, what is the role of mass ratio in this phase diagram?

We believe that changing the mass ratio $m_\mathrm{B}/m_\mathrm{F}$ would introduce only quantitative changes to the results of the present manuscript without changing the overall physical picture. Our belief is based on previous studies that considered generic mass ratios within the same formalism in 3D (Refs. 80 and 91, in particular). A more quantitative analysis supporting this statement would require performing the numerical calculations in 2D for generic masses. We stress that these numerical calculations are quite demanding. For this reason, as well as to avoid overloading the present work, we decided to focus here on equal masses. However, in view of possible future studies (by us or

other authors), we have developed the theoretical formalism and written all equations for generic masses. We have inserted a brief comment about this in the introduction (the last two sentences of the paragraph starting with "In this work, we study a 2D BF mixture in homogeneous space...").

15. At the end of section 2A where the quantum depletion is mentioned, I think a reference to condensation in a repulsive Bose gas would be helpful, or alternatively an explanation of what is meant by "quantum depletion determined by etaB"

We have reformulated the sentence mentioned by the Referee and quoted the paper by Schick (Ref. 94) that explicitly calculates the condensate depletion for a weakly repulsive 2D Bose gas.

16. Is the self-energy integral in Eq. 10 the same as the one introduced in Eq. 8? If yes, why not write SigmaB=Sigma11+ SigmaBF?

We have modified former Eq. 10 (now Eq. 11) as suggested by the Referee.

17. "The direct boson-boson repulsion is neglected in the present regime, since it is expected to produce negligible effect", I am guessing this is for realistic experimental values?

We actually meant that in the strong-coupling regime discussed in section 3, the (non-resonant) BB repulsion is expected to produce only minor effects. Physics is dominated by BF pairing and the corresponding large binding energy. We have slightly reformulated the sentence pointed out by the Referee in the revised version of our manuscript (see the two last sentences in the first paragraph of Sec. 3).

18. I could not find any detail as to how Eq. 19 and 20 were obtained exactly

We have provided details for the derivation of Eqs. 20-21 (former Eqs. 19-20) at the end of Appendix A, and referred to this derivation when introducing the above equations in Sec. 3.1.

19. Is there a simple expression for n0muF below Eq. 20?

We have added an explicit expression for $n^0_{\mu_F}$ below Eq. 21 (former Eq. 20).

20. When G0CF is introduced, should the reader know already what it is or is it simply a Green's function of the form in Eq. 21 which is rescaled to fulfill the frequency sum rule of Green's functions?

The paragraph containing former Eq. 21 (now Eq. 22) has been modified, together with the

subsequent paragraphs, also because of point 6 by the Referee. The quantity G^0_{CF} (which we now call $\tilde{G}^0_{\mathrm{CF}}$ because it contains a renormalized chemical potential $\tilde{\mu}_{\mathrm{CF}}$) is now defined explicitly by Eq. 24. So, there should be no ambiguities about its meaning.

21. Above Eq. 29 it is stated that the pole from G0B does not contribute. I am guessing this is due to the sign of the bosonic chemical potential. Was the sign of the bosonic potential already mentioned at this point? Does it ever change?

The Referee is right. We have added a comment above Eq. 35 (former Eq. 29) clarifying that the pole of G^0_B does not contribute because $\mu_B < 0$.

Concerning the question if the sign of μ_B can ever change, for BB repulsion $\eta_B = 0$ (considered in most of our calculations), μ_B is always negative due to the BF attractive interaction. For the alternative value $\eta_B = 0.1$, considered in some of our calculations, and $x \leq 1$, μ_B could become positive in the weak coupling limit $g \ll -1$ of the BF attraction. However, for the coupling strengths $g \geq -4$ considered in our calculations μ_B is always negative.

In the revised version of the paper, we have added information about the sign of μ_B after Eq. 5.

22. What does the sentence below Eq. 30 about neglecting Epm altogether with respect to muB mean?

Since in the strong coupling limit $-\mu_B \simeq \epsilon_0 \gg E_F$, it dominates over $E^{\pm}_{P=0}$, which is instead of order E_F. We have added a comment about it after Eq. 35 (former Eq. 30).

23. Section 3B, I feel it could be made clearer where small Delta0/EF is presumed and where one goes back to considering Eq. 32.

We think that the reorganization of section 3.2, following the advice at point 2 by the Referee, overcomes also this remark. Specifically, the details of the small Δ_0/E_F expansion have been moved to Appendix D.2, and the main equations resulting from this expansion are now reported at the end of section 3.2. In this way, we do not need now to go back to former Eq. 32 (now 38) afterward.

24. "Before passing to the exact evaluation of Eq. (32) in closed form, it is instructive for its physical interpretation to analyze the limit of small Delta0/EF, which is expected to occur either when x -> 1 (depletion of the condensate density due to increase of molecule number) or x-> 0

(reduction of the condensate density due to decrease of boson number)." How can this be understood intuitively? I understand that for x->0 we have nB->0 and since n0<nB we also have n0->0. But how can this be intuitively understood for x->1? If I understand correctly, then for all nB<nF, all bosons could potentially bind into molecules, leaving n0=0. Why is this only expected for x->1?

As already mentioned in our answer to point 2 by the Referee, even when n_0 exponentially vanishes for strong BF coupling, the hybridization energy $\Delta_0 \sim \sqrt{\varepsilon_0 n_0}$ may remain finite due to the large energy scale ε_0 (see new paragraph in sec 3.1 starting with "One sees from Eq. 29 ..." shortly after Eq. 29). As a matter of fact, only for $x \to 0$ or $x \to 1$, $\Delta_0 \to 0$ in the strong coupling limit, as can be seen from Fig. 3(b) and 14(b). We do not exclude that this picture could change in possible refinements of the present theory, but this is what one gets with the present approach.

25. I believe Eqs. 41,43 and 44 were never formally related to nF(k).

Former Eqs. 41,43, 44 have now been moved to appendix D.2, as suggested in point 3 by the Referee. They correspond now to Eqs. D.16, D.18, D.19, and are formally related to $n_F(k)$ immediately after Eq. D.19.

26. Why does the part in Eq. 45 that regards the population of composite fermions not have a corresponding theta function? Is there a way to understand Eqs. 45 and 46 in terms of two Fermi seas filling up? Or possible in terms of particle branches that are present in the two-body limit/ the non-interacting limit/ the Fermi polaron limit, which are then populated (albeit with modified quasiparticle properties)?

Former Eq. 45 (now Eq. 41) reports the momentum distribution of the fermionic atoms. These fermionic atoms can be unpaired or belong to composite fermions (paired states with bosons). The density of the fermionic atoms belonging to composite fermions is n_{CF} (since there is one atomic fermion for each composite fermion) and their momentum distribution is proportional (by the factor n_{CF}) to the square modulus of the molecular wave-function $|\phi(\mathbf{k})|^2$. We stress that the momentum $\mathbf{k}$ appearing in this term is the momentum of the fermion belonging to a composite fermion. It is not the center of mass momentum of the pair. For this reason, there is no theta function associated with the Fermi sphere of the composite fermion in front of this term in Eq. 41. The momentum

distribution function $n_{\rm CF}(\mathbf{P})$ for the center of mass momentum of the composite fermion is instead presented in sec. 3.1, and it is defined by Eq. 34 in the new version of the manuscript (see also Fig. 5). Therefore a representation in terms of atomic and molecular Fermi seas emerges via the quantities $n_{\rm UF}(\mathbf{k})$ and $n_{\rm CF}(\mathbf{P})$ presented in Secs. 3.2 and 3.1, respectively.

This point clearly emphasizes the importance of analyzing both two-particle and one-particle Green's functions for describing composite fermions and atomic fermions.

27. What is on the x-axis in the inset of Figure 3B? I presume x? I think Figure 3 would benefit from showing the condensate fraction.

We have added the missing label to the x-axis of the inset in Figure 3B. Additionally, we agree with the Referee that showing also the condensate fraction could be useful. We have added another inset reporting it in the same plot.

28. In the paragraph before the one starting with "In the crossover region, all chemical potentials are comparable in size", how can one understand the characterizations of the particle in terms of their chemical potentials? Is there an intuitive way to understand why for example $\tilde{\mu}_{\rm CF} > 0$ means degenerate molecules.

We have completely reformulated that paragraph, see two new paragraphs below Fig. 3 starting with "Two clearly different regimes can be distinguished in the opposite limits". Basically, the change in sign of the chemical potentials $\tilde{\mu}_{\rm CF}$ and $\mu_{\rm F}$ is identified as a proxy for the crossover region between two clearly distinct limits, in which the above chemical potentials have opposite sign, and nearly-free molecules or atomic fermions dominate the mixture, respectively.

29. I could not find it explicitly: Which method was used to obtain the results shown in Figure 3,4,5,6? Is it Eqs. 50-52 to obtain chemical potentials and condensate density or are additional Eqs. involved?

The Referee is correct: Figures 3,4,5,6 of Section 3.4 are obtained by solving the system of Equations 45-47 (former 50-52). We have now mentioned it explicitly at the end of the paragraph following Eq. 47. In addition, we already mentioned in the same paragraph that a standard root finder can easily solve the above system of equations. In particular, we used Mathematica's FindRoot function,

starting from reasonable values for the parameters.

30. "In Fig. 5 the quasi-particle weight nu2p of the occupied states Theta-E- is displayed for a number of concentrations corresponding to...". What does this mean? If I understand correctly then nu2p*Theta-E- is shown. In Figure 5, the qp-weight is also shown for unoccupied states, however for unoccupied states it is set to 0. That is not precisely the same thing. Similarly, in the caption of Figure 5 only nu2p is mentioned, but from Eq. 27 it is not clear to me that the function has a step-like drop (that only occurs after multiplying with Theta). Can this be formulated more precisely?

We thank the Referee for pointing out that the description of Fig. 5 was unclear. We have now introduced a formal definition for the momentum distribution of the composite fermions $n_{\mathrm{CF}}(\mathbf{P})$ in Eq. 34 of the revised manuscript, and have amended the caption of Fig. 5 and the text accordingly.

31. I think the paragraph below Figure 5 would benefit from explicitly stating what the Luttinger theorem is, how it breaks down, and how it is compensated in nCF. I am guessing Theta has larger support and in return nu2p is smaller, such that nCF remains constant?

We have now completely rewritten that paragraph and greatly expanded the discussion of the Luttinger theorem, quoting also several new references. We now state what the Luttinger theorem is, and discuss its extension to imbalanced Fermi systems and BF mixtures. We also discuss how it breaks down in our theory and provide an explanation for this breakdown.

For these changes, see in Sec. 3.4 the paragraph starting with "In Fig. 5 the momentum distribution", from the third sentence to the end of the paragraph, and the two new paragraphs that immediately follow it, which start with "The Luttinger theorem states" and "In a BF mixture with a condensate", respectively. Concerning the compensation of the breakdown of the Luttinger theorem in n_{CF} through the mechanism described by the Referee, it is commented in the paragraph starting with "Nevertheless, the breakdown of the Luttinger theorem". This paragraph was actually already present in the old version of our manuscript; we have only slightly modified it.

Finally, we now further discuss the breakdown of the Luttinger theorem in the same section when discussing Fig. 6, see the sentence starting with "We notice that this behavior, together with the one just discussed" and the paragraph that follows it.

32. Eq. 61 is first referenced below Figure 8, a long time before it is first introduced.

We now have moved former Eq. 61 (for the case $\eta_B = 0$ considered in Fig. 7) to Sec. 4.2 (Eq. 49 in the revised version of our paper).

33. I think more detail surrounding Eq.57 is needed. How can one see that a=1? What are the values of a, b as function of g? As is there is no real way to follow the argument made here.

We have added insets to Fig. 9 reporting the parameters a, b, and c as functions of g. Additionally, we now specify after Eq. 51 how the above parameters as a function of g have been obtained. Finally, we have created a data repository (Ref. 133) containing all data necessary to reproduce Figs. 3-15. The numerical values of the parameters a, b, and c are available in this repository.

34. "using the same thermodynamic parameters for both sets of curves". What does this mean? Same chemical potentials/condensate densities? If yes, how is this justified, shouldn't the different methods come up with different chemical potentials?

The comparison between the thermodynamic parameters (chemical potentials and condensate density) resulting from the full numerical calculation and from the strong-coupling expansion is made extensively in sections 4.3-4.5 (see Fig. 13-15, in particular). Here, in Fig. 11, we do something different. We focus *only* on the approximate expression 38 for $G_F(\mathbf{k}, \omega)$, from which Eq. 39 for $n_F(\mathbf{k})$ immediately results, and check to what extent it provides a good approximation for $G_F(\mathbf{k}, \omega)$, and thus $n_F(\mathbf{k})$. If, in doing this comparison, we would use in Eq. 38 the thermodynamic parameters resulting from the strong-coupling expansion (Eqs. 45-47) rather than the numerical ones, we would not check the validity of the approximate expression 38 alone, but also the validity of the approximations 46 and 47. As a matter of fact, one sees from Fig. 11 that the approximate expression 38 for $G_F(\mathbf{k}, \omega)$ is valid even for moderate values of the coupling strength ($g \simeq 1$). The comparison made in Sections 4.3-4.5 for the thermodynamic parameters shows instead that good agreement is found only for $g \gtrsim 2.5$. This indicates that the approximation 38 is valid in a more extended coupling range than the approximations 46 and 47, a piece of information that we believe might have some value.

In the revised version of our manuscript, we now explicitly explain the reason for our choice

of the thermodynamic parameters used in Fig. 11. See in Sec. 4.2 the paragraph starting with "Concerning the Fermi momentum distribution, we first discuss", containing the new sentences "to check to what extent the approximate expression ..." and "The use of the same thermodynamic parameters allows for ..."

35. "The boundary between them can be roughly estimated by looking at the smallest coupling at which muF vanishes as a function of x...". Is this a coincidence or is there physical meaning to muF=0? I guess this goes back to my question of how to characterize particles in terms of their chemical potentials.

This question is indeed related to point 28 and partly answered therein, as far as the fermionic chemical potential μ_F at $x \simeq 1$ is concerned. We have however decided to reformulate completely the paragraph containing the above sentence since, for generic concentrations, it is the bosonic chemical potential that yields more information on the crossover to the molecular limit, since the fermionic chemical potential is progressively less affected by interaction as the concentration is decreased. We believe that this new formulation is definitely clearer.

For the corresponding changes to the manuscript, see the new paragraph shortly after Eq. 55 "In particular, we have verified that for $g \simeq 1$ the relative difference ..,".

36. The notation in Eqs 60,61 can be confusing, I would suggest switching to nFk » kF(k) or something of that sort.

We have modified the notation in former Eqs. 60-61 (now Eqs. 56-57) as suggested by the Referee. We have consequently modified the notation also in Fig. 12.

37. I found it hard to follow what happens in Appendix B. I think a Feynman diagram would help.

We have added a Feynman diagram (Fig. 17), as suggested by the Referee.