Reply to Comment on ”Superfluid stability in the BEC-BCS crossover” by Sheehy and Radzihovsky

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Abstract

The reason behind the discrepancy between the phase diagrams of our earlier work [1] and the comment of Sheehy and Radzihovsky [2] is discussed. We show that, in contrast to what is claimed in [2], the requirement of positive susceptibility is sufficient to rule out states that are local maximum of the free energy (as a function of the order parameter \( \Delta \)).

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It is now widely accepted that, for an attractive s-wave interaction, an equally populated Fermi gas at zero temperature smoothly crosses over from the BCS to the BEC regime. In our recent paper \[1\], we considered a two component Fermi gas with unequal populations under a wide Feshbach resonance. We showed that the uniform state must become unstable at some intermediate coupling strength since it has either negative superfluid density or a negative susceptibility. Therefore we demonstrated that the smooth crossover known for the equal population case is destroyed (independent of the \textit{ansatz} what actually replaces the unstable states). A phase diagram was then constructed by indicating where the uniform state was found to be unstable (reproduced in Fig 1 here as the region between the dotted lines).

In a recent preprint, Sheehy and Radzihovsky \[2\] reinvestigated this phase diagram by a different method, and found discrepancy with our earlier results \[1\]. (see also \[4, 5, 6\]) In particular, they found that the instability region occupies a larger area than ours on the BEC side of the the phase diagram. They suggest that the susceptibility criterion \[3\] we used is not sufficient to rule out unstable states that are actually relative maximum of the free energy $\Omega$ with respect to the pairing potential $\Delta$.

We here would like to clarify the reason causing the discrepancy between the above two works \[1, 2\]. We now believe that our phase diagram in \[1\] is incorrect. However, the reason was in fact due to the inaccuracies of the numerical method we used there. Further, we argue that the susceptibility criterion is able to rule out states that corresponds to relative maxima of $\Omega$ (such as those depicted in Fig 2 of \[2\]), in contrast to what is claimed in \[2\].

First we comment on the method we used in \[1\]. A stable state must have all eigenvalues of the susceptibility matrix $\partial n_\sigma / \partial \mu_\sigma'$ positive (here $\sigma$ and $\sigma' = \uparrow, \downarrow$ for the two species, and $\mu_{\uparrow,(\downarrow)} = \mu \pm h$ are their chemical potentials and $n_\sigma$ are the densities). In \[1\], we solved, for the uniform states, the dimensionless average chemical potential $\tilde{\mu} \equiv \mu / \epsilon_F$ and potential difference $\tilde{h} \equiv h / \epsilon_F$ as a function of the dimensionless population difference $\tilde{n}_d \equiv n_d / n$ and coupling constant $g \equiv 1 / k_F a$. ($n = n_\uparrow + n_\downarrow, n_d = n_\uparrow - n_\downarrow$). The \textit{inverse} susceptibility matrix $\partial \mu_\sigma / \partial n_{\sigma'}$ can be expressed in terms of the above obtained functions \[1\]. It can further be shown \[7\] that a necessary condition that follows is that $\left( \partial \tilde{h} / \partial \tilde{n}_d \right)_g$ must be positive for stability, \textit{i.e.}, that the slope of $\tilde{h}$ versus $\tilde{n}_d$ must be positive at fixed scaled coupling constant $g$. Since the functions $\tilde{\mu}(\tilde{n}_d, g), \tilde{h}(\tilde{n}_d, g)$ were already available (see, e.g., Fig 1 of \[1\]), we chose to evaluate this matrix and its eigenvalues numerically from these data,
and constructed the phase diagram in [1]. Unfortunately, as we only found out later, the numerical accuracies required to carry out this method is very high, and we erroneously concluded in [1] that one of the eigenvalue changed sign at the same position as where \(\partial \tilde{h}/\partial \tilde{n}_d\) changed sign (footnote [13] of [1]). We have now re-evaluated the positions where (one of) the eigenvalue of this matrix changes sign more accurately, and the result is as shown as large circles in Fig 1 in this reply. As far as we can tell, this criterion yields the same line (dot-dashed) as where \(\partial^2 \Omega/\partial \Delta^2\) changes sign [8]. Thus on the left of this line, we find that our stable state has a positive susceptibility matrix as well as corresponds to a relative minimum of the free energy \(\Omega\), whereas on the right the unstable state identified has a susceptibility matrix with negative eigenvalue as well as corresponds to a relative maximum of the free energy \(\Omega\). Therefore, the susceptibility criterion is able to identify states that are relative maximum of the free energy and concludes that they are unstable, in contrast to what was claimed in [2].

The most transparent way to see the last statement is to consider the expression [9, 10]

\[
\left( \frac{\partial n_\sigma}{\partial \mu_{\sigma'}} \right) = \left( \frac{\partial n_\sigma}{\partial \mu_{\sigma'}} \right) + \frac{\left( \frac{\partial n_\sigma}{\partial \Delta} \right)_{\mu_\uparrow, \mu_\downarrow} \left( \frac{\partial n_{\sigma'}}{\partial \Delta} \right)_{\mu_\uparrow, \mu_\downarrow}}{\left( \frac{\partial^2 \Omega}{\partial \Delta^2} \right)_{\mu_\uparrow, \mu_\downarrow}} \quad (1)
\]

Note that the matrix \(\left( \frac{\partial n_\sigma}{\partial \mu_{\sigma'}} \right) \Delta\) has eigenvalues that are positive and finite (e.g. [2]), and the matrix \(\left( \frac{\partial n_\sigma}{\partial \Delta} \right)_{\mu_\uparrow, \mu_\downarrow} \left( \frac{\partial n_{\sigma'}}{\partial \Delta} \right)_{\mu_\uparrow, \mu_\downarrow}\) has non-negative eigenvalues. Consider now a stable state on the BEC side at large \(g\). This state has positive susceptibilities and is a free energy minimum, with \(\partial^2 \Omega/\partial \Delta^2 > 0\). Consider now decreasing \(g\), thus moving towards resonance. At the point where this state is no longer a free energy relative minimum but just becomes a relative maximum, \(\partial^2 \Omega/\partial \Delta^2 < 0\) and small. Thus the second term in eq (1), and therefore the susceptibility matrix itself, necessarily has a large and negative eigenvalue at this point. Therefore, as we claimed above, the susceptibility criterion is always able to identify the situation where, as coupling constant changes, a relative minimum becomes a relative maximum. (see also [5, 9])

We agree however with Sheehy and Radzihosky [2] that our susceptibility criterion may not always protect us from instability caused by a first order transition. But this can occur only when a new free energy minima arises at some other \(\Delta\), rather than having the original minimum turning into a relative maximum. In general, our criterion can fail when one can come up with a better ansatz for the state (at the same \(n\) and \(n_d\)) than the one
originally investigated, or there is a physical instability not contained in the susceptibility being evaluated. This happens in particular on the BCS side of the phase diagram [11]. To the right of the dotted line on the BCS side, the normal state is a free energy relative minimum. However, as suggested by the negative susceptibility matrix and superfluid density (for the latter, except near \( \tilde{n}_d \approx 1 \) of the uniform state to the left of this dotted line [1], a phase separated state and a state with finite pairing momentum (FFLO state) are potentially more stable than the normal state in a region near and to the right of this dotted line. One can straightforwardly evaluate these instability lines corresponding to these two ansatz. For phase separation, one finds the point where the free energy of the normal state becomes higher (when \( g \) is increased, i.e., moving from right to left in Fig 1) than that of the completely paired superfluid state (at the same chemical potentials \( \mu \) and \( h \) of the normal state). We evaluated the latter free energy by an integration over coupling constant [12]. The FFLO instability line of the normal state can be found by solving the Cooper problem at finite pair momentum \( q \), again at the chemical potentials of the corresponding normal state. These lines are also shown in Fig 1 here [13]. The diagram constructed from these transition lines then agree with [2] (see however the remark [11]).

In conclusion, we have resolved the discrepancy between the phase diagrams in [1] and [2]. The reason for the earlier disagreement was clarified.

While we were finishing the present manuscript, we noticed another preprint [14] discussing the same topic as here.

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[1] C.-H. Pao, S.-T. Wu and S.-K. Yip, Phys. Rev. B 73, 132506 (2006)
[2] D. E. Sheehy and L. Radzihovsky, cond-mat/0608172, see also cond-mat/0607803
[3] In this reply, we shall only mainly discuss the susceptibility since the requirement of positive superfluid density turns out to be weaker and so only the susceptibility condition is the subject of controversy with ref [2].
The inverse susceptibility matrix has elements \( B_{\sigma\sigma'} \equiv \left( \frac{\partial \mu_{\sigma}}{\partial \mu_{\sigma'}} \right) \). We have used the fact that in three dimensions, \( \epsilon_F \propto n^{2/3} \) and \( k_F \propto n^{1/3} \). The condition that all eigenvalues of \( B_{\sigma\sigma'} \) are positive requires that its expectation value with respect to the vector \((1, -1)\) be positive, and hence \( B_{\uparrow\uparrow} + B_{\downarrow\downarrow} - B_{\uparrow\downarrow} - B_{\downarrow\uparrow} > 0 \). Using the above expression for \( B_{\sigma\sigma'} \), we get the necessary condition \( \left( \frac{\partial \tilde{n}}{\partial \tilde{n}_d} \right) > 0 \).

Starting from the expectation value of the mean-field Hamiltonian in the gapless superfluid state, we get
\[
\frac{\partial^2 \Omega}{\partial \Delta^2} = \Delta^2 \sum_k \left[ \frac{1-f(E_k-h)}{E_k^2} + \frac{f'(E_k-h)}{E_k} \right]
\]
where \( E_k \)'s are the quasiparticle energies. (see also [5, 9])

In principle, this happens also on the BEC side of the phase diagram, as a first order phase transition also seems to occur there. A more correct phase transition line can be constructed using a procedure similar to Maxwell construction. However, the position of the phase transition line obtained by evaluating the susceptibility (or equivalently \( \frac{\partial^2 \Omega}{\partial \Delta^2} = 0 \), see also [5, 9]) turns out to be almost exactly the same as that given in [2] (see also [3, 4]) and thus the correction needed to the transition line on the BEC side in Fig 1 is rather small.
FIG. 1: (color online) The phase diagram, with the region where the uniform state being unstable shaded. The stable region to the BCS (right) side corresponds to the normal state, whereas the one on the BEC (left) side corresponds to a gapless superfluid. The boundaries for the unstable region reported in [1] are indicated by the dotted lines. On the BEC side, the dot-dashed line represents where $\frac{\partial^2 \Omega}{\partial \Delta^2}$ changes sign. Circles are where an eigenvalue of the susceptibility matrix changes sign. On the BCS side, the dashed (blue) line represents the location where the normal state becomes unstable towards phase separation. The full (red) line represents the finite $q$ Cooperon instability of the normal state.