Ultracold polarized Fermi gas at intermediate temperatures

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We consider non-zero temperature properties of the polarized two-component Fermi gas. We point out that stable polarized paired states which are more stable than their phase separated counterparts with unpolarized superfluid region can exist below the critical temperature. We also solve the system behavior in a trap using the local density approximation and find gradually increasing polarization in the center of the system as the temperature is increased. However, in the strongly interacting region the central polarization increases most rapidly close to the mean-field critical temperature, which is known to be substantially higher than the critical temperature for superfluidity. This indicates that most of the phase separation occurs in the fluctuation region prior to superfluidity and that the polarization in the actual superfluid is modest.

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I. INTRODUCTION

Since their experimental realization the properties of the strongly interacting superfluid Fermi gases have been studied ever more actively. In particular the recent experiments have probed the properties of fermion pairing in a novel settings. Some important theoretical contributions appeared before the breakthrough in a polarized two-component Fermi system of trapped ultra cold gases have probed the properties of fermion pairing in a novel settings. Some important theoretical contributions appeared before the breakthrough experiments motivated a series of theoretical works which have explained various features of the experiments with non-rotating gases in the low temperature regime.

Since the BCS-phase cannot support polarization at zero temperature, one typically expects, in a harmonic trap, phase separation into an unpolarized superfluid core, surrounded by the polarized normal Fermi gases. The transition between the phases is sharp in the local density approximation (LDA) and local minimization of the grand potential rules out the possibility of the local maxima of the free energy, known as the Sarma or breack-pair (BP) state. LDA approach can, however, be modified to include a possibility for a BP phase if one minimizes the total (global) energy of the system. Such modification can in principle predict a ring of BP phase in the boundary region where BCS phase is transformed into the normal phase, and for large polarization, BP phase is also found in the center of the trap. In this paper we will assume that these boundary effects are small and can be ignored. For a system in which the number of fermions is very large and the trap does not have a too high aspect ratio, this is expected to be a good approximation although it is quite likely that these boundary terms are important in defining the largest possible polarization that can still support a superfluid.

While the above described works consider mainly zero temperature, we now concentrate on finite temperature effects. In a work fairly closely related to ours Machida et al. considered the finite temperature effects by solving the mean-field Bogoliubov-de Gennes equations numerically in a cylinder with a harmonic trap in the radial direction. Qualitative picture they find is in many places similar to ours, although the simple local density approximation we apply in a trap is insufficient to properly describe the regions they call “FFLO” phase. Also a very recent work by Chien et al. investigated the superfluid properties of the homogeneous polarized Fermi gas across the BEC-BCS cross-over also at non-zero temperatures. At intermediate temperature regime they found that stable polarized Fermi superfluids are possible. Various aspects of finite temperature effects in BEC-BCS cross-over were also recently discussed by Yi and Duan.

The purpose of this paper is to point out that polarized BCS states, when they exist, also have a lower energy than the corresponding phase separated state with an (finite temperature) unpolarized paired part and polarized normal part. Furthermore, using LDA we find the state of the system in a trap as a function of temperature and find that the system becomes gradually polarized in the center of the trap. Since this occurs also at temperatures still well below the critical temperature we expect the mean-field theory employed here to provide at least qualitatively valid description of the system. However, most rapid increase of the central polarization occurs in the fluctuation region above the superfluid transition temperature. This indicates that most of the phase separation in the trapped system would occur prior to the onset of superfluidity.

This paper is organized as follows. In Sec. II we discuss the uniform BCS phase and compute how highly polarized such a state could be. In Sec. III we proceed to compare the energies of the polarized BCS phase with the mixed phase of unpolarized BCS phase and a polarized normal gas. In Sec. IV we investigate the intermediate
temperature properties in a trapped gas using the local density approximation. We end with some concluding remarks in Sec. III.

II. POLARIZED UNIFORM DENSITY BCS STATE

The grand potential corresponding to the standard mean-field BCS theory of interacting two component Fermi can be computed from the mean-field Hamiltonian

\[ H = \sum_{k,\sigma} [\epsilon_k - \mu_\sigma] \hat{\psi}_k^{\dagger} \hat{\psi}_k - \frac{\Delta}{2} \sum_k \left( \hat{\psi}_{k,2}^{\dagger} \hat{\psi}_{k,1}^{\dagger} + \hat{\psi}_{k,1} \hat{\psi}_{k,-2} \right) + \frac{\Delta^2}{g}, \]

where \( \hat{\psi}_{k,\sigma} \) is the (fermionic) annihilation operator for species \( \sigma \) and the coupling strength \( g = 4\pi\hbar^2a/m \) is expressed in terms of the scattering length \( a \). Furthermore, \( \Delta = g \langle \hat{\psi}_1(r) \hat{\psi}_2(r) \rangle \) is the order parameter/gap function, which we take to be independent of position, \( \epsilon_k = \hbar^2 k^2/2m \) is the free dispersion, and \( \mu_\sigma \) is the chemical potential for the \( \sigma \)-component. Since we are going to apply this Hamiltonian also in the strongly interacting regime, some phenomenological model building is clearly involved. In particular, the existence of a non-zero gap function should not be taken as an indicator of superfluidity. Superfluidity would imply phase stiffness and this typically occurs at a lower temperature \([31, 32]\) than the mean-field critical temperature predicted by the above Hamiltonian.

The assumption of a constant gap function is in this context quite reasonable, but it does rule out the possibility of the FFLO-phases \([33, 34]\), which could in principle exist in some narrow range of parameters \([17]\). Diagonalizing the above Hamiltonian we can simply calculate the grand canonical free energy

\[ \Omega(\mu_1, \mu_2, \Delta) = -k_B T \log[\text{Tr}(\exp(-\beta H))], \]

as a function of temperature \( T \) \([27]\). Due to the use of the interaction interaction the resulting expression is ultraviolet divergent and this divergence is removed by the usual renormalization

\[ \frac{\Delta^2}{g} \to \frac{\Delta^2}{g} - \frac{1}{V} \sum_k \frac{\Delta^2}{2\epsilon_k} \]

where \( V \) is the quantization volume which drops out from the final physical results. The gap equation can be derived from the grand potential as condition for the extrema \( \partial \Omega / \partial \Delta = 0 \), while the number equation appears from \( n_\sigma = -\partial \Omega / \partial \mu_\sigma \), where \( n_\sigma \) is the component density. Alternatively, the latter condition can be enforced as an extremal point of the Helmholtz free energy \( F = \Omega + \mu_1 n_1 + \mu_2 n_2 \), i.e. \( \partial F / \partial \mu_\sigma = 0 \). In this section we choose the units using the ideal Fermi gas of density \( \bar{n} \) as a benchmark and \( \bar{n} \) is taken to be an average of the component densities. This means that the unit of length is given by \( l = 1/k_F = (6\pi^2 \bar{n})^{-1/3} \), while the unit of energy is \( \epsilon_F = \hbar^2 k_F^2 / 2m \).

The polarized BCS solution corresponds to the minimum of the grand canonical free energy, but does not exist at zero temperature. At zero temperature only stationary points of the free energy corresponding to the polarized solutions and spatially constant gap are the normal state and the BP state. However, as the temperature is increased stable polarized BCS solutions can appear.

In Fig. 1 we show the largest possible polarization \( p_c(T) = (n_1 - n_2) / (n_1 + n_2) \) with a large and moderate coupling strength. It is clear that BCS solutions corresponding to the minimum of the grand potential with substantial polarizations do exist in the strongly interacting regime as the temperature increases. For very weak interactions the polarization supported becomes vanishingly small, but the maximum polarization of the BCS state can be as high as \( p_c(T) \approx 0.68 \) in the strongly interacting regime with \( k_F a = -100 \). If the polarization is higher than this the system will never enter a uniform superfluid region as the temperature is lowered towards \( T = 0 \). Curiously, this critical density asymmetry is close to the experimentally observed critical atom number asymmetry in a trap \([15]\).

Naturally close to critical temperature of the mean-field theory the approach used here becomes unreliable, but states of considerable polarization do exist even well below the critical temperature. The maximum polarization supported by the BCS state is predicted to peak in the intermediate temperature regime. This is expected since the critical temperature is maximized in an unpolarized system and therefore just below the critical temperature only small polarization is possible.

![FIG. 1: The highest value of polarization that the uniform BCS state can support as a function of temperature (in units of Fermi temperature) when \( k_F a = -100 \) (solid line) and \( k_F a = -1 \) (dashed line). We have set the maximum polarization equal to zero in the region above the critical temperature.]
III. PHASE SEPARATED STATE VS. POLARIZED BCS STATE

Let us now turn to the possibility of phase separation. At zero temperature the phase separated state is clearly favored since the polarized BCS solution does not exist. However, as we saw in the previous section at non-zero temperature the polarized BCS solutions do exist and it is not clear if these polarized BCS states have a lower energy than the phase separated state corresponding to the same number of atoms.

In particular, we have in mind a comparison with an unpolarized BCS phase occupying a volume fraction $1 - x$ ($0 \leq x \leq 1$) next to a polarized normal phase in a volume fraction $x$. If the unpolarized BCS phase has a density $n_{BCS}$ the normal state will have fermion densities

$$n_{\sigma,n} = \frac{n_{\sigma} - (1 - x)n_{BCS}}{x}$$

if the average density for each component, averaged over the whole the system, is $n_{\sigma}$. The problem is then to find the values of $x$ and $n_{BCS}$ which minimize the Helmholtz free energy $F(x, n_{BCS})$ for given set of parameters, such as coupling strength, polarization, and temperature. When the interface energy is ignored the Helmholtz free energy is simply a sum of two contributions, the polarized normal gas and unpolarized BCS phase.

In Fig. 2 we show how the optimum normal state volume fraction behaves as a function of polarization in a phase separated state at zero temperature. Quite sensibly, for weaker interactions the normal part increases faster with polarization while in the strongly interacting regime the paired part persists longer. Our result for weaker interaction appears to be consistent with the earlier result by Bedaque et al.\[35\]. As we increase the temperature the normal part will become bigger and eventually at the critical temperature we have a phase transition into a pure normal state.

Since our approach does not include surface energy contribution from the boundary between superfluid and normal regions, the zero temperature transition to a fully normal state as polarization increases is not sharp. Nevertheless, the volume fraction of the paired region becomes so close to zero that it drops below our numerical resolution. If one were to include the surface terms\[36\], one would expect a sharp boundary as well as a shift downwards from the “critical” polarization around $p = 0.85$ for the stronger interactions.

In Fig. 3 we show the minimum attainable Helmholtz free energy as a function of temperature for the phase separated state, together with the energies of the polarized BCS state, and the pure normal state with fixed polarization of 0.1 in the strongly interacting regime. While the energy differences are not large, it is nevertheless clear that whenever the (stable) polarized paired state exists, it is more stable than the phase separated state. Furthermore, the energy of the phase separated state is an underestimate due to the absence of the surface energy contributions. The mean-field theory used here ignores some fluctuations contributions to the free energy, but we believe these are not going to change the outcome of the energy comparison since these contributions would have to be included in both competing states. This outcome is made all the more likely by the absence of surface energy contributions in the phase separated state.
IV. LOCAL DENSITY APPROXIMATION AT $T \neq 0$

At zero temperature, for an ideal Fermi gas we find in the local density approximation a component density

$$n_{\sigma}(r) = \frac{1}{6\pi^2} \left[ \frac{2m}{\hbar^2} \left( \mu_{\sigma} - V_T(r) \right) \right]^{3/2},$$

(5)

where the external trapping potential is given by $V_T(r) = m\omega^2 r^2 / 2$ and the component chemical potential $\mu_{\sigma}$ is related to the particle number $N_{\sigma}$ through $\mu_{\sigma} = \hbar\omega (6N_{\sigma})^{1/3}$. The density vanishes outside the Thomas-Fermi radius $R_{TF,\sigma} = \sqrt{2\mu_{\sigma}/m\omega^2}$. The polarization $p_N = (n_1 - n_2)/(n_1 + n_2)$ will then be

$$p_N(r) = \frac{(\mu_1 - V_T(r))^{3/2} - (\mu_2 - V_T(r))^{3/2}}{(\mu_1 - V_T(r))^{3/2} + (\mu_2 - V_T(r))^{3/2}}$$

(6)

inside the Thomas-Fermi radius of the minority component. This implies that for an ideal gas the polarization will increase from

$$p_N(r = 0) = \frac{1 - \sqrt{N_2/N_1}}{1 + \sqrt{N_2/N_1}}$$

(7)

in the center of the trap to the maximum value of $p_N(r > R_{TF,2}) = 1$ beyond the Thomas-Fermi radius of the minority component.

On the other hand at zero temperature superfluid one expects strong phase separation due to the absence of the polarized superfluid state corresponding to the minimum of the grand potential. In that case, if we ignore the boundary effects, we would find vanishing polarization $p_S(r)$ in the center of the cloud, which then abruptly increases close to the trap edge, eventually becoming $p_S(r > R_{TF,2}) = 1$ beyond the Thomas-Fermi radius of the minority component.

As we have found, the paired polarized state can exist at non-zero temperature and furthermore when it exists it has a lower energy than the corresponding phase separated state with non-polarized superfluid mixed with a normal Fermi gas. This then raises the question of what the polarization $p(r)$ will be in a trap at intermediate temperatures. Finite temperature effects will round off the density distribution and make the LDA analysis less accurate, but we expect it to be qualitatively valid. Also, since the mean-field theory of the strongly interacting Fermi gas becomes more unreliable at higher temperatures, it appears fruitless to aim towards higher precision within the framework of the mean-field theory.

Since the energy of the polarized BCS state increases with polarization it will be energetically more favorable to have a large number of atoms in a region of fairly small polarization, rather than forming, for example, a small core of highly polarized superfluid surrounded by the normal gas or perhaps unpolarized BCS phase. This implies, quite sensibly, that $p(r)$ will be something in between the normal state polarization $p_N(r)$ and the $T = 0$ phase separated superfluid polarization $p_S(r)$.

The normal state polarization increases smoothly up to 1 and as we have found, the BCS state can be polarized if the (local) polarization is below the critical value $p_\sigma(T)$. Also one expects that the extent of the (possibly) polarized superfluid core becomes smaller as the temperature is increased and eventually disappears at a critical temperature where polarized BCS states can no longer be found. Outside the paired core one expects a polarized normal Fermi gas. These qualitative arguments are quite well confirmed by solving the state of the system using LDA analysis. This implies using the local chemical potentials $\mu_{eff,\sigma} = \mu_{\sigma} - V_T(r)$ and finding $\mu_{\sigma}$ in such a way that the total particle numbers have the desired values. At non-zero temperatures the contributions from $\mu_{eff,\sigma} < 0$ do not vanish identically and the edge of the cloud is rounded somewhat by this effect.

In Fig. 4 we show a typical result for the densities, the gap, as well as the density difference as a function of position and temperature in the strongly interacting regime with a number asymmetry $(N_1 - N_2)/(N_1 + N_2) = 0.5$. The behavior of the gap function is qualitatively similar even if the paired region were polarized. The spatial extent of the paired core first, somewhat surprisingly, increases slightly as the temperature increases, but is then reduced as one approaches the critical temperature. This effect is however so small, that it would be difficult to observe and could be an artifact of the LDA. At zero temperature LDA analysis gives rise to abrupt changes in densities (especially for the minority component) and also the gap drops suddenly to zero. Increasing temperature eventually removes all these discontinuities. As the temperature is lowered below the critical temperature the minority component develops a clear bimodal density distribution.

The polarization as a function of position naturally becomes different as the temperature increases due to the appearance of polarization in the paired core. The polarization in the center of the cloud increases gradually with increasing temperature, but this build-up becomes more abrupt if the number asymmetry increases. If fluctuations were to be included, the critical temperature for the superfluidity could become so low (in the strongly interaction region) that the actual superfluid region would have only a small polarization. The build-up of polarization and removal of phase separation with increasing temperature would therefore mostly occur in the “pseudo-gap” region. For more weakly interacting system this distinction disappears, but then also the polarization that the BCS state can carry drops and the superfluid region will again have only a small polarization.

Qualitatively the behavior predicted by the LDA does not change strongly when the number asymmetry is increased to 0.8. Interestingly, it turns out that the position dependence of the local polarization $[n_1(r) - n_2(r)]/[n_1(r) + n_2(r)]$ becomes weaker as the temperature increases. This suggests that approximating the system as uniform, might not always be too dra-
A gradual appearance of the polarized superfluid as the Fermi gas. The LDA approach used here predicts an almost identical signature on the integrated density distribution of the Fermi gas of strongly interacting regime is naturally questionable especially at non-zero temperatures and is expected to give rise, for example, to a substantial overestimate of the critical temperature for superfluidity. Therefore, the critical temperature found here provides an estimate on the temperature when pairing effects appear, but not necessarily on the superfluid transition temperature when phase coherence sets in. The results presented here in the strongly interacting region are qualitatively similar in the weakly interacting regime where the fluctuations are less strong. The absolute magnitudes of the possible polarizations, the superfluid gap, and the critical temperature are then, however, substantially smaller.

At zero temperature it is known from the Monte-Carlo calculations that the mean-field theory overestimates the gap substantially. In order to provide more accurate quantitative predictions it would therefore be important to understand the intermediate temperature properties of strongly interacting Fermi gases better. This is all the more important due to the very recent MIT experiment which observed prominent interaction effects close to and somewhat above the (superfluid) transition temperature and also pointed out the need of incorporating the interaction effects between the normal and superfluid regions into a quantitatively accurate theory.

FIG. 4: (a) The pairing gap, (b)-(c) component densities, and (d) the density difference as a function of position and temperature. The result is calculated in the strongly interacting regime with coupling strength $k_F a = -20$ and number asymmetry $(N_1 - N_2)/(N_1 + N_2) = 0.5$. The unit of energy is the Fermi energy $\epsilon_F = \hbar^2 k_F^2/2m$ of the ideal Fermi gas of $^6$Li atoms with $(N_1 + N_2)/2 = 10^5$ atoms in a harmonic trap with $2\pi (\omega_x \omega_y \omega_z)^{1/3} = 600$ Hz. Unit of length is $1/k_F$ and densities are scaled with the factor $6\pi^2$ so that ideal gas would have a density of $n_{ideal} = 1$ in the center.

FIG. 5: (a) The doubly integrated density difference $\Delta n(z) = \int dx dy [n_1(x, y) - n_2(x, y)]$ at $T = 0$ (solid) and $T = 0.2$ (dashed). The result is calculated with same parameters and units as in Fig. 4. (b) The column integrated density difference $\Delta n(z, y = 0) = \int dx [n_1(x, y = 0, z) - n_2(x, y = 0, z)]$ at $T = 0$ (solid) and $T = 0.2$ (dashed). The result is calculated with same parameters and units as in Fig. 4.

V. SUMMARY AND CONCLUSIONS

In this paper we have employed the mean-field theory at finite temperatures to discuss the behavior of the interacting Fermi gases with unequal numbers of fermions in two components. We found that stable polarized paired states can exist at intermediate temperatures and that cross-over to a polarized paired state can leave a moderate signature on the integrated density distribution of the Fermi gas. The LDA approach used here predicts a gradual appearance of the polarized superfluid as the temperature is increased.

The accuracy of the mean-field theory in the strongly interacting regime is naturally questionable especially at non-zero temperatures and is expected to give rise, for

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