Heat capacity of a two-component superfluid Fermi gas

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Abstract

We investigate mean-field effects in two-component trapped Fermi gases in the superfluid phase, in the vicinity of $s$-wave Feshbach resonances. Within the resonance superfluidity approach we calculate the ground state energy and the heat capacity as function of temperature. Heat capacity is analyzed for different trap aspect ratios. We find that trap anisotropy is an important factor in determining both the value of heat capacity near the transition temperature and the transition temperature itself.
At present several groups [1, 2, 3] have produced Fermi gases of atoms at temperatures where the superfluid phase is expected. The possibility of tuning interatomic interactions near Feshbach resonances may provide a chance to watch macroscopic phenomena for both normal and superfluid phases and the phase transition from one to another. The presently reachable temperatures limit the existence of the superfluid phase to a strongly-interacting gas. For now it is still an open question how to observe the superfluid transition, although numerous proposals exist [4, 5, 6, 7, 8, 9] (and references therein).

Here we examine the thermodynamics of a two-component Fermi gas in a strongly-interacting regime where we can expect superfluidity. Although any attractive interaction can theoretically support Cooper pairing at zero temperature, it seems that only a strongly-attractive interaction may produce observable effects in current experiments. For a strongly-interacting gas the 'small parameter' $k_Fa > 1$ and so the ordinary mean-field approach breaks down. In this case the resonance superfluidity [10, 11, 12] approach suits the problem best. On the experimental side the strongly-interacting regime is reached by exploiting magnetic-field Feshbach resonances [1, 2, 3]. For our numerical simulation we took the parameters of the two-component Fermi gas of $^{40}K$ near Feshbach resonance. These components are in $|\frac{9}{2} - \frac{9}{2} >$ and $|\frac{9}{2} - \frac{5}{2} >$ states. In [1] it was shown that there is an s-wave Feshbach resonance at a magnetic field $224.21 \pm 0.05$G and near this resonance the scattering length was measured up to about $\pm 2000a_0$.

Kokkelmans et al [11] employed the resonance superfluidity approach in order to get the critical temperature and find possible signs of the phase transition. Ohashi and Griffin [12] independently used the same approach. For the superfluid phase we use the mean-field approach of BCS-type theory within the local density approximation and use the Hamiltonian of the resonance superfluidity model [11] in order to take Feshbach resonance physics into account. In this case the energy density functional $\mathcal{E}$ depends on normal $\rho(x, y)$, anomalous $\kappa(x, y)$ densities and a molecular field $\phi(\frac{x+y}{2})$ where $x$ and $y$ are coordinates of two atoms. The set of equations as well as their solution for energy-independent effective interaction (see [13] for example) look like in ordinary Bogolyubov-de Gennes formulation but with the extra term of a molecular field:

$$\rho(k, R) = n(k, R)v^2(k, R) + (1 - n(k, R))v^2(k, R),$$
$$\kappa(k, R) = u(k, R)v(k, R)(1 - 2n(k, R))$$
\[
E(k, R) = \sqrt{h(k, R)^2 + \Delta(R)^2},
\]
\[
\begin{pmatrix}
 u^2(k, R) \\
 v^2(k, R)
\end{pmatrix} = \frac{1}{2} \left(1 \pm \frac{h(k, R)}{E(k, R)}\right)
\]
\[
h(k, R) = \frac{\hbar^2 k^2}{2m} + V_{mf}(R) + V_{trap}(R) - \lambda
\]

where \(k\) is a wavevector, \(R = \frac{x+y}{2}\) is the coordinate of the center of the mass for two interacting atoms, \(n(k, R) = (e^{E(k, R)/k_B T} + 1)^{-1}\) is the Fermi-Dirac distribution, \(V_{mf}(R)\) is a mean field potential and \(\Delta(R)\) is the energy gap. \(V_{bg} = 4\pi \hbar^2 a_{bg}/m, a_{bg}\) is the background scattering length, \(g = \sqrt{V_{bg} \Delta B \Delta \mu}\) is the coupling strength and, \(\nu = (B - B_0) \Delta \mu\) is the magnetic field detuning, \(\Delta B\) is the field width of the resonance, \(\Delta \mu\) is the magnetic moment difference between two hyperfine levels of the two-component Fermi gas \([11, 15]\).

More complete theoretical analysis using this approach can be found in \([12]\). Functions \(f(k, R)\) are the Wigner transforms of corresponding functions \(f(x, y)\). So after solving (1) we have both a normal \(\rho(k, R)\) and an anomalous \(\kappa(k, R)\) distribution function as well as the molecular field \(\phi(R)\) and we find the ground state energy as:

\[
E = \int \frac{d^3 k}{(2\pi)^3} \int d^3 R \left\{k^2 \rho(k, R) + V_{bg} \rho(k, R) \rho(R) + \rho(k, R) 2V_{trap}(R) - \Delta(R) \kappa^*(k, R) \right\}
\]

\[
+ \int d^3 R V_{trap}^{mol}(R) \phi^2(R)
\]

It is a well-known phenomenon that near the phase transition the energy-temperature curve should have a distinct change. Moreover we can investigate the dependence of specific heat capacity and ground state energy on interaction strength and trap aspect ratio. As we will see the geometry of the trap strongly influences the thermodynamics of the superfluid gas.

We consider an anisotropic trap with trap aspect ratio \(\lambda = \omega_z/\omega_\perp\) of the transverse and axial frequencies. Because the ratio \(\lambda\) is rather small in the current experiments \((\approx 0.01)\) \([1,2]\) calculations for isotropic or almost isotropic traps possess only a methodological interest. However, it is in nearly isotropic traps that the most dramatic observables are
expected; see below. As the interaction near a Feshbach resonance strongly depends on detuning we consider all the characteristics of this system as a function of detuning $\nu$ and temperature $T$. For present calculations we chose $\omega_\perp = 400Hz$ and $5 \times 10^5$ particles. As the detuning is defined by the magnitude of a magnetic field we will report detuning in units of Gauss, which is more convenient for a possible comparison with experiment.

Within this approach we have calculated the ground state energy and heat capacity for a variety of interactions and temperatures. The typical dependence of ground state energy and gap on detuning is shown in Fig.(1, 2). In the range of detuning shown the interaction is always attractive so a superfluid phase can exist. But at a detuning larger than $\approx 1G$ the pairing energy seems rather small compared to the kinetic energy as the energy-detuning dependence is very weak. In the vicinity of a resonance the mean-field $V_{mf}$ contribution to the ground state energy is negligible as the background part of the scattering length is small compared to the resonance part. With decreasing detuning the pairing energy becomes a significant part of the total energy and we can see considerable lowering of the total energy beginning from some detuning that depends on temperature too. Unfortunately it is impossible to estimate the kinetic and the pairing energies separately because the integral of the second and forth terms in (2) over momentum are individually divergent [16].

Fig.1 thus shows that detunings smaller than $\approx 1G$ seem required to observe superfluidity. In Fig.1 the solid curves are calculations for $\lambda = 0.5$. The dotted curves are for $\lambda = 0.05; 0.01$ and for $T = 0.1T_F$. So for more anisotropic traps the pairing energy is smaller. It should be possible to measure the energy, as in [17]. In [17] the released energy was measured for Bose gas above and below the transition temperature. The uncertainty is $\approx 10 – 30\%$ for temperatures below $T_c$. The desired detuning should therefore be small enough to generate at least a $10\%$ change in energy compared to the normal phase energy. Thus the detuning should be smaller than $0.5G$ for $T/T_F = 0.1$, $\lambda = 0.5$. For more realistic trap aspect ratios (0.01) it should be smaller than $0.3G$ At these values of detuning the pairing energy is not a small part of the total ground state energy which means that the energy gap is rather large too (Fig. 2).

From experimental point of view it seems that the closer to the resonance we are the more chances to observe superfluidity we have. But it should be mentioned that near a resonance there is so called the BCS-BEC crossover regime [18]. In theory of the superconductivity at this regime there is a class of ‘exotic’, high-$T_c$ superconductors. In the case of the crossover
regime \((\mu/\Delta \leq 1)\) we need a more sophisticated theoretical\(^{19}\) approach than the ordinary mean-field theory. Such a treatment is outside of scope of the present article, but it may be important in order to get the right value of the critical temperature \(^{20}\) for this regime. If \(\mu/\Delta\) is sufficiently greater than 1 we can hope we have the ordinary BCS regime. For smaller trap ratios the condition \((\mu = \Delta)\) happens at a slightly smaller detunings.

In this article we do not analyze how much larger \(\mu/\Delta\) should be for the theory to hold, and leave such an analysis for the near future. So for further investigations we have chosen detunings \(\nu = 0.3 - 0.5G\) where the energy gap is still significant. The energy-temperature dependence (Fig. 3) is a more appropriate characteristic for the comparison and describing of experimental data. Again from an experimental uncertainty point of view it seems that temperatures around 0.1\(T_F\) or smaller are more appropriate to observe superfluidity. For chosen parameters of interest we have the condition \(\Delta \gg \hbar \omega\) and according to the pairing classification of \(^{14}\) this is an inter-shell pairing regime for which the local density approximation is the appropriate tool for describing the pairing.

The important characteristic of the pairing field is its distribution in momentum \(\kappa(k, R)\) (Fig. 4). In the same figure we demonstrate this distribution for \(\nu = 0.4; 1G\) (dashed and dotted curves) for \(T = 0.1T_F\). Far from resonance \((\nu = 1G,\) dashed line\) this function has just a narrow peak near Fermi momentum \(k_F\). With decreasing detuning more and more atoms below \(k_F\) are involved in the pairing which emerges not only as a Fermi surface effect. As it was shown in \(^{21}\) the product \(k_F\xi\) (\(\xi\)- the coherence length) is the appropriate variable for ‘exotic’ superconductors. Moreover the value \(\xi\) can be considered as the size of the Cooper pair. Within our approach the coherence length is dependent on location \(\xi^2(R) = \int d\kappa\langle r, R \rangle r^2/ \int d\kappa\langle r, R \rangle \approx (k_F(R)/m\pi\Delta(R))^2\). We have calculated this for the center of the trap and found that \(\xi\) is about 0.33-1.65 in trap units for \(\nu = 0.3 - 0.5G\) and \(\lambda = 0.01\) But the interparticle distance is changing much slower and is around 0.35 for the given detunings. For our reasonable detunings and \(\lambda = 0.01\) the parameter \(k_F\xi\) is 2-26-8 but the ‘boundary’ which distinguishes the high-\(T_c\) and conventional superconductors \(^{21}\) is \(k_F\xi \approx 2\pi\). It was suggested \(^{22}\) that the ‘exotic’ superconductors are intermediate between BCS-type superconductors and BEC. Holland et al \(^{10}\) predicted the same phenomenon for the two-component degenerate Fermi gas. So according to this classification we have conventional superfluidity for \(\nu \approx 0.5G\) and larger. Moreover at this field \(k_F a < 1\) and the ordinary mean-field theory can be used.
The coherence length can give us an insight into whether it is possible to detect a signal of the Cooper pair breaking, similar to what was done for bound molecular states at negative magnetic-field detunings [23]. If it is possible, this can be considered as a sign of superfluidity. From this point of view it seems that it is not desirable to be very close to resonance because in this case the many-body wave function of the Cooper pair at distances of the coherent length order between atoms will be very close to the two-body wave function for quasi-bound states near a resonance. At large distances between atoms the wave function of the Cooper pair will be very different from the relative wave function of two scattering atoms but it is not clear if the RF spectroscopy can work at such distances. Our approach enables us to find the Cooper pair wave function and in the future we will analyze this aspect in more detail.

The phase transition to superfluidity stipulates a considerable increase in heat capacity near the critical temperature. This characteristic may therefore serve as an observable sign of superfluidity. The main point of the present article is an investigation of a heat capacity for Fermi gas for the conditions described above. In [24] the authors calculated and analyzed this characteristic for off-resonance interacting $^6$Li within ordinary HFB theory and the effect is too small to be detected in current experiments. But the resonance superfluidity approach gives us a chance to do this analysis for strongly-interacting systems. The phenomenon of superfluidity strongly depends on the trap geometry. For an s-wave interacting gas the $R-$dependence on the energy gap $\Pi$ reflects only the trap geometry. In our calculations we keep $\omega_\perp = 400Hz$ and vary $\omega_z$. It is clear that with decreasing $\lambda$ the energy gap will be smaller in the center of the trap than for an isotropic trap. So the spatial manifestation of the superfluid phase $\Pi$ depends on geometry too.

We found (Fig. 5, 6) that the trap anisotropy considerably influences the heat capacity of a gas in the superfluid phase and can wash out the effect altogether if $\lambda$ is very small. It is known that at the critical temperature the heat capacity has a discontinuity. In the trap-confined gas the $T_c$ as well as the gap is $R$-dependent and the higher the temperature is, the smaller is the fraction of the gas involved in superfluidity. The critical temperature is the point at which the energy gap disappears in the center of the trap. Above this temperature the gas is in the normal phase everywhere. We can see that for temperatures lower then $T_c$ heat capacity of the superfluid phase can be up to $\approx 1.5$ times larger than for normal phase gas, and this value depends on the trap aspect ratio and detuning. Also the more
anisotropic a trap is the smaller the gap is and then smaller a 'bump' in heat capacity for superfluid phase.

The heat capacity as well as the energy of ground state can be measured using a ballistic expansion as was done for a Bose gas [17]. But, as it was pointed out in [1, 2] an expanding strongly-interacting gas is likely in the hydrodynamic regime. We have estimated that for temperatures near the critical temperature and at small detunings (0.2-0.4G) the collision rate [1, 2] can be larger than the trap frequency, which also depends on the trap aspect ratio. It means that the hydrodynamic regime is very probable during the expansion. We can choose the trap aspect ratio in order to get the collision rate a bit smaller than the transverse frequency. For $\nu = 0.3G$ at the corresponding critical temperature the ratio $\lambda$ should be around 0.01(Fig. 5). A similar estimation for $\nu = 0.4G$ shows that $\lambda$ can be around 0.05(Fig. 6). It is clear that for reasonable parameters near the resonance the cloud will not be expanded ballistically as a whole. However, a measurement of the total energy after turning-off the trap is still valid, since the released energy should be conserved. The trap energy is almost two times smaller than total energy so the energy-temperature dependence of the released energy will be very similar to that shown in Fig. 3 but approximately two times smaller.

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FIG. 1: Ground state energy per particle as a function of the detuning for different temperatures. The temperature is in $T_F$ units. The trap aspect ratio $\lambda = 0.5$ for the solid curves. The dotted curves display different aspect ratios for $T = 0.1T_F$. 
FIG. 2: Energy gap in the center of the trap and chemical potential as a function of the detuning for different temperatures. $\lambda = 0.5$. 
FIG. 3: Ground state energy per particle as a function of a temperature for the magnetic field detuning $\nu = 0.2 - 0.6G$ with step $= 0.1G$ The dotted line is the energy in the case when the interaction is described just by the non-resonant scattering length.
FIG. 4: Distribution function $\kappa(k, R=0)$ in the center of the trap versus momentum for the pairing field for different temperatures in the case $\nu = 0.2G$ and $\lambda = 0.01$. Also shown are the cases for $\nu = 0.4$(dotted line) and $\nu = 1G$(dashed line) and for $T = 0.1T_F$. 


FIG. 5: Heat capacity as a function of a temperature for detuning \( \nu = 0.3G \) and for different trap aspect ratios \( \lambda \). The dashed line is for the normal phase gas.
FIG. 6: Heat capacity as a function of a temperature for detuning $\nu = 0.4G$ and for different trap aspect ratios $\lambda$. The dashed line is for the normal phase gas.