Detection of the BCS transition of a trapped Fermi Gas

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We investigate theoretically the properties of a trapped gas of fermionic atoms in both the normal and the superfluid phases. Our analysis, which accounts for the shell structure of the normal phase spectrum, identifies two observables which are sensitive to the presence of the superfluid: the response of the gas to a modulation of the trapping frequency, and the heat capacity. Our results are discussed in the context of experiments on trapped Fermi gases.

The observation of Bose-Einstein condensation in several atomic systems [1] has recently sparked increasing interest in trapped fermionic atoms. These systems offer the prospect of a Bardeen-Cooper-Schrieffer (BCS) transition to a superfluid phase at low temperatures \( T < T_c \). By trapping the atoms in two hyperfine states, the phase transition temperature \( T_c \) should be experimentally accessible [2,3], and several experimental groups are presently working to achieve this transition [4,5]. However, as only a few percent of the atoms are likely to participate in Cooper pairing [6], it is not obvious how the transition could be observed in these dilute systems. Recently, it has been proposed that the propagation and scattering of light should be significantly altered by the presence of Cooper pairs [7,8]. Since the quasiparticles (QP) with energies near the Fermi chemical potential, \( \mu_F \), are those most affected by the Cooper pairing, candidate observables for the detection of the BCS transition should be sought from phenomena sensitive to this low-energy region of the QP spectrum.

In this paper, we consider two such observables: the response of the gas to a “shaking” of the trap, as first suggested by Baranov [9]; and the heat capacity. For low \( T \), both of these observables are dominated by contributions from the low-energy spectrum. By presenting a complete calculation of the properties of the trapped gas in both the normal and superfluid phases, which accounts exactly for the quantization of the single-particle energy levels, we are able to predict if these two observables are suitable to detect the presence of Cooper pairing. Our analysis should have direct relevance to the ongoing experiments on trapped Fermi gases.

We consider a gas of fermions of mass \( m \), confined by a potential \( U_0(\mathbf{r}) \), with an equal number of atoms \( N_\sigma \) in each of two hyperfine states, \( |\sigma| = \pm \). Two fermions in the same internal state \( \sigma \) must have odd relative orbital angular momentum (minimally \( p \)-wave), and at low temperatures the centrifugal barrier suppresses their mutual interaction [10]. Thus, we suppose the interaction to be effective only between atoms in different hyperfine states and to be dominated by the \( s \)-wave contribution. As the interplay between the discrete nature of the normal phase spectrum and the Cooper pairing is crucial for the quantities considered in this paper, we need a theory which can describe the interaction and Cooper pairing of atoms residing in different discrete trap levels. This precludes the use of a simple Thomas-Fermi treatment [11]. A theory appropriate for the present paper has recently been presented [12]. It uses a zero-range pseudopotential [13] to model the interaction between atoms in two different hyperfine states; this is appropriate when the scattering length for binary atomic collisions, \( a \), has a larger magnitude than the effective range of the interaction, \( r_e \), and when \( k_F|a| \ll 1 \), where \( k_F = \sqrt{2m\mu_F}/\hbar \) is the Fermi wavevector. The generalized mean field theory derived from this approach yields the eigenvalue problem [12]:

\[
E_\eta u_\eta(\mathbf{r}) = \left\{ \hat{\mathcal{H}}_0 + W(\mathbf{r}) \right\} u_\eta(\mathbf{r}) + \Delta(\mathbf{r}) v_\eta(\mathbf{r})
\]

\[
E_\eta v_\eta(\mathbf{r}) = -\left\{ \hat{\mathcal{H}}_0 + W(\mathbf{r}) \right\} v_\eta(\mathbf{r}) + \Delta(\mathbf{r}) u_\eta(\mathbf{r}).
\]

Here \( \hat{\mathcal{H}}_0 = \frac{-\hbar^2}{2m} \nabla^2 + U_0(\mathbf{r}) - \mu_F \) is the single-particle Hamiltonian; \( W(\mathbf{r}) \equiv g(\hat{\psi}_+(\mathbf{r})\hat{\psi}_-(\mathbf{r}))/\hbar \) is the Hartree potential, where \( \hat{\psi}_\sigma(\mathbf{r}) \) is the atom field operator for component \( \sigma \) at position \( \mathbf{r} \), which obeys the usual fermion anticommutation relations. The coupling constant is \( g = 4\pi a k^2/m \) and the pairing field, \( \Delta(\mathbf{R}) \), is defined by

\[
\Delta(\mathbf{R}) = -g \lim_{r \to 0} \partial_r r\left( \hat{\psi}_+(\mathbf{R} + \frac{\mathbf{r}}{2})\hat{\psi}_-(\mathbf{R} - \frac{\mathbf{r}}{2}) \right).
\]

Our definition of the pairing field differs from that often employed in weak-coupling BCS theory [14]. The main advantage of the definition given above is that it eliminates the ultraviolet divergence present in the usual weak-coupling theory [13]. The elementary quasiparticles (QP’s) with excitation energies \( E_\eta \) are described by the Bogoliubov wave functions \( u_\eta(\mathbf{r}) \) and \( v_\eta(\mathbf{r}) \).

We solve the Bogoliubov-de Gennes (BdG) equations [14] for the case of an isotropic harmonic potential, \( U_0(\mathbf{r}) = m\omega^2r^2/2 \), using a self-consistent numerical procedure outlined elsewhere [12]. In the absence of the pairing field, the QPs exhibit a discrete spectrum of energies \( E_\eta \), with the index \( \eta \) designating a triple of quantum numbers \( (n, l, m) \), where \( l, m \) are the usual angular momentum quantum numbers and \( n \) is an index of radial excitation. In the presence of the pairing field, the self-consistent solution to the BdG equations with the lowest free energy is spherically symmetric. Thus, the Bogoliubov wavefunctions are given by \( u_\eta(\mathbf{r}) = r^{-1}u_{nl}(\theta)Y_{lm}(\theta, \phi) \) and \( v_\eta(\mathbf{r}) = r^{-1}v_{nl}(\theta)Y_{lm}(\theta, \phi) \), where the \( Y_{lm} \) are the usual spherical harmonics, and with \( n, l, m \) being implicitly indexed.
by \( \eta \). The paring field, which is a scalar operator under rotations, couples a normal phase QP with \((n, l, m)\) to one with \((n', l, -m)\). Due to the spherical symmetry, in taking sums over states needed to obtain the results of this paper, we can replace sums over \(m\) by factors of \((2l + 1)\).

We now calculate the response of the gas to a harmonic time-dependent perturbation of the trapping potential, \( \Delta H(t) \), of the form

\[
\Delta H(t) = \lambda \sin(\tilde{\omega}t) \sum_n \int d^3r \frac{1}{2} m \omega^2 r^2 \psi_n^*(r) \psi_n(r),
\]

where \( \lambda \) is a small parameter. We expand the field operators in terms of the Bogoliubov wave functions and the QP operators in the usual way \[14\], and by applying Fermi’s golden rule to obtain the linear response \( R(\tilde{\omega}) \) of the gas to the perturbation, Eq. (3), we obtain:

\[
R(\tilde{\omega}) \propto 2 \sum_{n \neq n'} (2l + 1) \int_0^\infty dr (u_{nl}^* u_{n'l} - v_{nl} v_{n'l})^2 \times (f_{nl'} - f_{nl}) \delta(\hbar \tilde{\omega} + E_{nl'} - E_{nl}) + \sum_{n \neq n'} (2l + 1) \int_0^\infty dr (u_{nl}^* u_{n'l} + v_{nl} v_{n'l})^2 \times (1 - f_{nl'} - f_{nl}) \delta(\hbar \tilde{\omega} - E_{nl'} - E_{nl}),
\]

where \( f_{nl} = (\exp \beta E_{nl} + 1)^{-1}, \beta = 1/k_B T, \) and \( k_B \) is Boltzmann’s factor. The physical interpretation of the two terms in Eq. (4) is straightforward: The first term describes the excitation of a QP due to the perturbation, whereas the second term describes the creation of two QPs. This latter process does not violate particle conservation, since the QPs in general are mixtures of real particles and holes. The response of the gas should be observable as density fluctuations of the trapped gas. As we have assumed a spherical symmetric perturbation, the transitions all have \( \Delta l = 0 \). A generalization to perturbations with arbitrary angular momentum \( l \) is straightforward. In the non-interacting limit, Eq. (4) reduces to a sum of delta functions \( \delta(\tilde{\omega} - 2n\hbar \omega) \) with \( n = 0, 1, 2, \ldots \).

We now solve the BdG equations self-consistently and then calculate the response of the gas to a “shaking” of the trap from Eq. (4). In Fig. 2, we show a typical plot of the response \( R(\tilde{\omega}) \) for various values of \( T' = k_B T / \hbar \omega \). In this example, we have chosen the parameters \( \mu / (\hbar \omega)^2 = -0.8 \) and \( \mu_F = 51.5 \hbar \omega \), where \( \hbar = (\hbar / m \omega)^1/2 \) is the characteristic length of the ground-state harmonic oscillator wavefunction. With the value of \( a = -2160a_0 \), appropriate to \(^6\)Li \[14\], these parameters correspond to \( N \sim 3 \times 10^4 \) atoms of each spin state in a trap with frequency \( \nu = \omega / 2\pi \approx 520 \text{Hz} \); a value of \( T_c \approx 5.6 \hbar \omega / k_B = 140 \text{mK} \) for the transition temperature is obtained by linearizing Eq. (4). Fig. 2 shows the response for \( T' = 0 \), 3.95 and 4.55, where the gas is in the superfluid phase, and for \( T' = 0 > T_c \), where the gas is in the normal phase. For comparison, we also plot the \( T = 0 \) response, assuming the gas is in the normal phase. Each delta function in Eq. (4) representing a \( t \to \infty \) resonance, is smoothed out to a frequency range of \( \sim \omega / 10 \) to model the finite frequency resolution of the appropriate experiment.

We now discuss these results, considering first the response for the normal phase. The resonance peaks for \( T = 0 \) and \( T' = 0 \) are relatively narrow on the scale of \( \omega \). This is perhaps surprising, as one might expect the Hartree field to wash out the shell-structure of the QP spectrum in the normal phase \[10\]. To understand this, we plot in Fig. 2 the lowest QP energies \( E_{l\eta} \) for the gas in the normal phase at \( T = 0 \). To simplify the plot, we include only even values of \( l \). The QP energies with odd \( l \) behave in a completely analogous way. All energies are positive; negative normal-phase particle energies are simply holes \((u_{nl} = 0)\) with positive energy in this representation. For \( T = 0 \), only the \( \delta(h \tilde{\omega} - E_{l\eta} - E_{l'n'}) \) term in Eq. (4) is non-zero. The thick vertical arrow in Fig. 2 indicates a typical transition: creation of a hole with energy \( E_{n'h} \), and a particle with energy \( E_{n''p} \), yielding \( h \tilde{\omega} = E_{n'h} + E_{n''p} \simeq 2.2 \hbar \omega \). The analysis of this normal-phase spectrum is basically the same as the one presented in Ref. \[10\]. A key result of the present paper is the finding that, although the Hartree field has introduced a significant dispersion of the QP energies as a function of \( l \), the dispersion is almost the same for each band. Hence, for \( \Delta l = 0 \), the difference of energies between two particle bands (or the sum of energies of a particle and a hole band, as in Fig. 2) varies much less with \( l \) than the energies themselves, which results in a relatively narrow resonance peak. The resonance for \( T = 0 \) is sharper than for \( T' = 0 \). This is because for \( T = 0 \), only the energy bands immediately around \( \mu_F \) contribute to the response due to the Fermi exclusion principle, whereas for higher \( T \), there are transitions between several bands that yield slightly different transition energies.

We now consider the response when the gas is in the superfluid phase. By comparing the result for \( T' = 6 \) and \( T' = 4.55 \) in Fig. 3, we see that when the gas enters the superfluid phase, there is a significant broadening of the resonance line. This is due to the fact that Cooper pairing starts to mix particles with holes, and the QP spectrum is altered. This is depicted in Fig. 3, which shows the lowest even-\( l \) QP levels for \( T' = 4.55 \) for both superfluid and normal phases. When the energies of particles and holes are almost degenerate in the normal phase (\( l \sim 26 \) in Fig. 3), the pairing strongly mixes these two states. This leads to the usual avoided crossing and the QP spectrum is changed significantly. The strong mixing yields the broadening of the resonance line depicted in Fig. 3. There are now transitions with significantly lower energies than in the normal phase. Such a transition, which contributes to the \( \delta(h \tilde{\omega} - E_{l'n'} - E_{l\eta}) \) term in Eq. (4) with \( E_{l\eta} - E_{l'n'} \simeq 0.8 \hbar \omega \), is indicated by the vertical arrow in Fig. 3. We also note that the effect of the pairing decreases with increasing \( l \). This is simply because the centrifugal potential “pushes” the high \( l \)
states into the region where the order parameter becomes very small. The inset in Fig. 4 shows $\Delta(r)$ and $|W(r)|$. For $T' = 4.55$, the pairing only takes place around the center of the cloud, and QP states which have a small amplitude in this region are unaffected.

For $T \ll T_c$, all the low lying QP states are strongly influenced by the pairing. From the inset in Fig. 4, we see that Cooper pairing now takes place over the entire trapped cloud. The low energy QP spectrum for $T = 0$ plotted in Fig. 4 is qualitatively different from the normal phase spectrum. The low energy QP wave functions are centered between the regions where the pairing field and the trapping potential are significant. These “in-gap” states, which were first discussed by Baranov [1], depend strongly upon the strength of pairing. As $T$ decreases and $\Delta(r)$ increases, their energy increases. The response of the gas is completely dominated by these states for $T \ll T_c$. The broad peak for $T = 0$ in Fig. 4 comes from the $\delta(\hbar \omega - E_\sigma - E_p)$ term in Eq. (4) with $E_p = E_p$ being the lowest energy for a given $l$. It reflects excitations of the kind $\gamma^{\dagger}_{\eta \sigma} \gamma_{\eta \sigma} |\Phi_0\rangle$ where $|\Phi_0\rangle$ is the ground state and $\gamma^{\dagger}_{\eta \sigma}$ creates a QP with quantum numbers $\eta$ in hyperfine state $\sigma$. Hence, for $T \ll T_c$ the response of the gas is a broad peak coming from excitations of the lowest QP band. The resonance peak should be centered around an increasing frequency as $T$ is lowered, since $\Delta(r)$ increases. This is confirmed in Fig. 4, where a broad peak has emerged in the response for $T = 3.95$, the peak being centered at a lower frequency than for $T = 0$.

The qualitative behavior of the response of the gas described above depends on the fact that the resonance peaks are relatively well-defined in the normal phase. We have performed a number of calculations varying both the coupling strength and the number of atoms trapped. For experimentally realistic parameters, it turns out that the Hartree field does not wash out the resonance peaks in the normal phase. We therefore believe the analysis above should be valid for typical experimental conditions.

The low-$T$ heat capacity is another observable which probes the low lying QP spectrum. The usual way to measure the energy of a trapped gas is to turn off the trapping potential and then deduce the velocity distribution from the expanding cloud [1,7]. As the trapping potential is turned off non-adiabatically, the velocity distribution has a $\delta(\hbar \omega - E_\sigma - E_p)$ term in Eq. (4) with $E_p = E_p$ being the lowest energy for a given $l$. It reflects excitations of the kind $\gamma^{\dagger}_{\eta \sigma} \gamma_{\eta \sigma} |\Phi_0\rangle$ where $|\Phi_0\rangle$ is the ground state and $\gamma^{\dagger}_{\eta \sigma}$ creates a QP with quantum numbers $\eta$ in hyperfine state $\sigma$. Hence, for $T \ll T_c$ the response of the gas is a broad peak coming from excitations of the lowest QP band. The resonance peak should be centered around an increasing frequency as $T$ is lowered, since $\Delta(r)$ increases. This is confirmed in Fig. 4, where a broad peak has emerged in the response for $T = 3.95$, the peak being centered at a lower frequency than for $T = 0$.

To conclude, we have presented a detailed analysis of two possible ways of detecting the predicted BCS phase transition for a trapped gas of fermionic atoms. The onset of Cooper pairing influences significantly the response of the gas to modulation of the trapping frequency. For $T > T_c$, the response has a relatively sharp peak, and the width of the peak should narrow as $T$ is lowered. Then as $T = T_c$ is reached, one should observe a significant broadening of the response peak as the Cooper pairing starts to affect the low lying QP spectrum. For $T \ll T_c$, the low lying QP states are qualitatively different from the normal phase states, and the response of the gas to the shaking is predicted to be a broad peak coming from the lowest QP band. The center of the peak should move to increasing frequencies as the pairing increases for decreasing $T$. Also, one should be able to detect the phase transition by looking at the low $T$ heat capacity. It should be exponentially suppressed for $T \ll T_c$, reflecting the gapped nature of the QP spectrum due to Cooper pairing. However, a measurement of the heat capacity is destructive as one has to release the trap and it requires several repetitions of the trapping experiment. Also, the suppression of $C_{N_{\alpha}}$ is only significant for $T \ll T_c$. We therefore estimate that it is a less direct way of detecting the transition than by looking at the response to a modulation of the trapping frequency. The analysis presented
here should be qualitatively correct for a non-spherical symmetric trap as well, although the actual calculations would be more cumbersome in this case.

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FIG. 1. The response $R$ of the gas as a function of the modulation frequency $\tilde{\omega}$ for various temperatures. The inset shows the Hartree field $|W(r)|$ (dot-dashed) and $\Delta(r)$ for $T' = 0$ (solid) and $T' = 4.55$ (dashed) in units of $\hbar\omega$.

FIG. 2. The lowest QP energies in units of $\hbar\omega$ at $T = 0$ for the normal phase ($\times$) and the superfluid phase (Solid line).

FIG. 3. The lowest QP energies in units of $\hbar\omega$ at $T' = 4.55$ for the normal phase ($\times$) and the superfluid phase (Solid line).
FIG. 4. The heat capacity in units of $k_B$ for the normal (dashed) and the superfluid (solid) phase.