Optical detection of a BCS transition of Lithium–6 in harmonic traps

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Abstract. – We study the detection of a BCS transition within a sample of Lithium–6 atoms confined in a harmonic trap. Using the local density approximation we calculate the pair correlation function in the normal and superfluid state at zero temperature. We show that the softening of the Fermi hole associated with a BCS transition leads to an observable increase in the intensity of off–resonant light scattered from the atomic cloud at small angles.

The experimental realization of Bose-Einstein-Condensation in dilute Alkali vapors stimulated a variety of experimental and theoretical work in the field of quantum gases. Recently, attention was also drawn to the special properties of ultracold fermionic gases. In particular the absence of a $s$–wave scattering interaction in a spin polarized system would allow to realize an almost perfect example of a noninteracting Fermi gas, of which first indications were observed in an experiment with $^{40}$K atoms. In the case of an attractive interaction between different hyperfine levels as occurs in $^6$Li, the ground state will be a BCS superfluid. Stoof et al. first proposed to look for this phase transition in a mixture of two hyperfine states of $^6$Li, where due to the extraordinary large $s$–wave scattering length the transition temperature turns out to be in an observable range of about 100nK. Their work was further expanded by Modawi and Leggett, including all three hyperfine states that can simultaneously be enclosed in a magnetic trap.

An experimental realization of the BCS–transition in magnetic traps is aggravated by particular conditions regarding the life time of the sample, equal occupation of the hyperfine states and a large magnetic offset field to obtain the maximal scattering length of $a = -1140\,\text{Å}$ for lithium, so that cooling of the sample in a pure optical trap might be advantageous. Besides these difficulties, the most favorable way to detect a BCS–transition in future experiments is still a matter of discussion. In fact, the differences in the density and momentum distribution between the normal and superfluid phases are tiny, so that unlike the case of bosonic gases, time–of–flight measurements will not be able to indicate the phase transition. As possible observable signatures collective excitations, changes in the line width and line shift in
light scattering experiments \cite{10} and anomalous moments of inertia \cite{11} have been suggested. In this paper we show that the BCS transition in a cloud of cold atoms may be detected directly by off-resonant light scattering. This suggestion was made independently by Zhang et al. \cite{12}, however our results for the signature of the transition are quite different from theirs, see our discussion at the end of the paper. Recent measurements of the dynamic structure factor in Bose condensates \cite{13} show that even the time dependent pair correlation functions have indeed become accessible by experiments.

We consider a system of fermionic atoms in two equally occupied hyperfine states trapped in an isotropic harmonic potential \( V(x) = \frac{1}{2} m \omega^2 x^2 \). Atoms in different hyperfine states interact via an attractive contact interaction \( V(x, y) = V_0 \delta(x - y) \). The corresponding Hamiltonian is

\[
\hat{H} = \sum_{\sigma} \int d^3 x \, \Psi^\dagger_{\sigma}(x) \mathcal{H}_0 \Psi_{\sigma}(x) + \frac{V_0}{2} \sum_{\sigma} \int d^3 x \, \Psi^\dagger_{\sigma}(x) \Psi^\dagger_{-\sigma}(x) \Psi_{-\sigma}(x) \Psi_{\sigma}(x). \tag{1}
\]

where \( \Psi_{\sigma}(x) \) is a fermionic field operator which destroys a particle in hyperfine state \( \sigma \) at location \( x \) and \( \mathcal{H}_0 = -\hbar^2/2m \nabla^2 + V(x) - \mu \) denotes the single particle Hamiltonian. The diagonalization of this Hamilton operator in mean field approximation is equivalent to solving the Bogoliubov–de Gennes equations, originally formulated for inhomogeneous superconductors \cite{14}

\[
E_k u_k(x) = [\mathcal{H}_0 + W(x)] u_k(x) + \Delta(x) v_k(x) \tag{2}
\]

\[
E_k v_k(x) = -[\mathcal{H}_0 + W(x)] v_k(x) + \Delta(x) u_k(x). \tag{3}
\]

Here we introduced the Hartree potential \( W(x) = V_0 \langle \Psi^\dagger_{\sigma}(x) \Psi_{\sigma}(x) \rangle \) and the pair potential \( \Delta(x) = -V_0 \langle \Psi_{\sigma}(x) \Psi_{-\sigma}(x) \rangle \), which both depend on the position in the trap. As in the conventional BCS theory the function \( v_k(x) \) can be interpreted as the amplitude for the occupation of a Cooper pair with excitation energy \( E_k \). The amplitudes are normalized by

\[
\sum_k (u_k(x) u_k^*(y) + v_k(x) v_k^*(y)) = \delta(x - y). \tag{4}
\]

We will not attempt to provide a complete solution of these equations which is quite involved numerically and also requires a nontrivial regularization procedure for the pseudo potential \cite{15}. Instead, we use the local density approximation (LDA), which relies on the fact that both the Fermi wavelength \( \lambda_F \) and the BCS coherence length \( \xi_0 \) are much smaller than the typical scale \( x_0 = \sqrt{\hbar/m \omega} \), on which the harmonic external potential varies. The results of the LDA can be obtained from the Bogoliubov–de Gennes equations by using an ansatz \( u_k(x) = \exp(i k x) \hat{u}_k(x) \), \( v_k(x) = \exp(i k x) \hat{v}_k(x) \) with slowly varying amplitudes \( \hat{u}_k(x) \), \( \hat{v}_k(x) \). Inserting this into the Bogoliubov–de Gennes equations and neglecting all derivatives of \( \hat{u}_k(x) \) and \( \hat{v}_k(x) \), the excitation energy is the familiar \( E_k(x) = \sqrt{(\xi_k(x) - \mu(x))^2 + \Delta^2(x)} \) with the local chemical potential \( \mu(x) = \mu - V(x) - W(x) \). Similarly the amplitudes take the standard BCS form

\[
\hat{u}_k(x) = \sqrt{\frac{\xi_k(x)}{2 E_k(x)}} \left( 1 + \frac{\xi_k(x)}{E_k(x)} \right) \frac{1}{2}, \quad \hat{v}_k(x) = \sqrt{\frac{\xi_k(x)}{2 E_k(x)}} \left( 1 - \frac{\xi_k(x)}{E_k(x)} \right). \tag{5}
\]

\(^{(1)}\)The LDA can also be interpreted as the semi-classical \( \hbar \to 0 \) limit of an Ansatz \( u_k(x) = e^{i p x / \hbar} \hat{u}_k(x) \).
with the reduced single particle energies $\xi_k(x) = \varepsilon_k - \mu(x)$. In order to determine the local values of $\mu(x)$ and $\Delta(x)$ we numerically solve the standard gap equation together with that for the total number of particles. The ultraviolet divergence in the gap equation which arises from the assumption of a contact potential with no extrinsic cutoff in energy of the attractive interaction, can be eliminated by using the standard relation between the bare interaction parameter $V_0$ and the low energy effective interaction $g = 4\pi\hbar^2a/m$, which is determined by the scattering length $a$. The resulting density distribution and local pair potential are in very good agreement with those found earlier [7, 11, 15], with a typical cloud radius $R_T \approx v_F/\omega$.

For particle numbers of order $6 \cdot 10^3$ used in our calculations, the LDA is in fact an excellent approximation as was shown by Bruun et al. [15].

We now turn to the calculation of the pair correlation function. Using the Wick–theorem the pair correlation function $g(x, y)$ separates into a normal part $g^N(x, y)$ and an anomalous part $g^A(x, y)$:

$$g(x, y) = \langle \hat{n}(x)\hat{n}(y) \rangle - \langle \hat{n}(x) \rangle \langle \hat{n}(y) \rangle = g^N(x, y) + g^A(x, y).$$  \hspace{1cm} (6)

The normal part correlation function consists of the autocorrelation part and the anti–correlation between fermions in the same spin states. The anomalous correlation function is nonzero only in the superfluid phase, when anomalous expectation values occur due to the formation of pairs. At zero temperature and within the LDA the normal and anomalous parts of the correlation function are given by

$$g^N(x, y) = n(x)\delta(x - y) - 2 \left( \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(x - y)}\tilde{\nu}_k(x)\tilde{\nu}_k(y) \right)^2. \hspace{1cm} (7)$$

$$g^A(x, y) = 2F(x, y)F^*(y, x). \hspace{1cm} (8)$$

where $F(x, y)$ is the anomalous pair amplitude

$$F(x, y) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(x - y)}\tilde{\nu}_k(x)\tilde{\nu}_k(y). \hspace{1cm} (9)$$

The pair amplitude diverges for $r = |x - y| \to 0$ like $m\Delta(y)/4\pi\hbar^2r$, which is an artefact of the zero range interaction. Unlike the pair potential this divergence cannot be compensated by a divergence in the coupling constant. A rough estimate for the local pair correlator is obtained by taking $F(x, x) = \Delta(x)/g$ with $g$ as the renormalized interaction constant, leading to

$$g(x, x) = -\frac{n^2(x)}{2} + 2\frac{\Delta^2(x)}{g^2}. \hspace{1cm} (10)$$

While the scattered intensity calculated below is rather insensitive to the precise value of $g(x, x)$, this relation shows explicitly that the positive anomalous correlations associated with a BCS–transition reduce the effect of the Fermi hole in the pair correlation function of fermions.

In the normal state, where $\Delta(x) = 0$, the anomalous correlations vanish and we obtain the following inhomogeneous generalization of a well–known result for Fermi gases:

$$g^N(x, y) = n(z)\delta(r) - \frac{1}{2} \left[ \frac{3n(z)}{(k_F(z)r)^2} \left( \sin(k_F(z)r) - k_F(z)r \cos(k_F(z)r) \right) \right]^2. \hspace{1cm} (11)$$
Fig. 1. – The scattering geometry used in this paper: A monochromatic light beam with wave vector \( \mathbf{k} \) scatters at the atomic trap placed at the origin. In a minimal distance \( z_0 \) from the trap an observation screen is placed. The scattered intensity is measured at distance \( R_\perp \) from the center of the observation screen.

Here we introduced \( z = \text{Max}(x, y) \), \( r = |x - y| \) and the local Fermi wave vector \( k_F(z) = \sqrt{2m\mu(z)/\hbar^2} \). The correlation function shows the typical Friedel oscillations with period \( \lambda_F/2 \) and an algebraic decay \( r^{-4} \) caused by the Fourier transform of the step in the Fermi distribution at zero temperature. In the superfluid regime with \( \Delta(x) \neq 0 \), the pair correlations can only be calculated numerically. Reflecting the tiny differences of the density distributions, the normal correlation functions differ only at large distances, where their absolute values are negligible.

The anomalous correlation function also exhibits Friedel oscillations and an exponential decay on a scale \( k_F^{-1} \). Naively one would expect a decay with the BCS coherence length \( \xi_0 = \hbar v_F/\Delta_0 \) as in the homogeneous case, but the inhomogeneity of the amplitudes \( \tilde{u}_k(x) \) and \( \tilde{v}_k(x) \) blocks this effect. Overall, the magnitude of the anomalous correlation function is about 10% of the normal correlations although it is formally a very small effect of order \( (\Delta_0/\varepsilon_F)^2 \approx 0.01 \) for realistic parameters in \(^6\text{Li}\).

In the following, we will see that due to an almost perfect cancellation of the autocorrelation and the normal correlation contributions in an off–resonance light scattering experiment, the effect of the anomalous correlations is quite appreciable. The scattering geometry is shown in Figure 1. The incoming laser beam with amplitude \( E_L \) and wave vector \( k \) produces an atomic polarization \( \mathbf{P}(\mathbf{r}) \) which for a large detuning \( \delta \) of the laser frequency from the resonance is given by

\[
P(\mathbf{r}) = -\frac{d^2E(\mathbf{r})}{\hbar \delta}n(\mathbf{r}).
\] (12)

Here \( d \) is the matrix element of the atomic dipole moment and \( n(\mathbf{r}) \) the gas density in the trap. We calculate the scattered field \( \mathbf{E}_{sc} \) in first order Born approximation. Assuming that the incoming laser field is removed by the dark ground technique and neglecting the temporal variation due to the excitation processes, the measured intensity at position \( R_\perp \) on the screen is given by

\[
I(\mathbf{R}) = \langle \mathbf{E}_{sc}(\mathbf{R})\mathbf{E}_{sc}(\mathbf{R}) \rangle = \frac{9I_L}{16(kR^2\delta)}(F_n(R_\perp) + F_c(R_\perp)),
\] (13)
where \( I_L \) is the laser intensity. The first contribution to the intensity is essentially the Fourier transform of the density distribution in the trap

\[
F_n(R\perp) = \left| \int d^3r \ e^{ik(\hat{R} - \hat{e}_z) \cdot r} n(r) \right|^2. \tag{14}
\]

where \( \hat{R} \) and \( \hat{e}_z \) are unit vectors in the direction of \( R \) and in \( z \)-direction respectively. The second contribution to the intensity contains the pair correlation function:

\[
F_c(R\perp) = \int \int d^3r \ d^3r' \ e^{ik(\hat{R} - \hat{e}_z) \cdot (r - r')} g(r, r'). \tag{15}
\]

The contribution \( F_n(R\perp) \) can be described as simple coherent scattering from a circular hole with an amplitude proportional to \( N^2 \) and indeed our numerical results show the typical Bessel function behaviour [18]. From the first minimum in the scattered intensity, which occurs at \( 1.22 R\lambda/d \), we can extract an effective radius \( d/2 \) of the circular opening. Due to the variation of the density through the atomic cloud this radius turns out to be about half the Thomas–Fermi radius \( R_T \) of the trap. For the numerical calculations we use a trap frequency \( \omega = 2\pi \times 144 \text{Hz} \) and chemical potential \( \mu_0 = 110.5 \hbar \omega \) as typical parameters [7]. This corresponds to an oscillator length of \( x_0 \approx 3.4 \mu m \), a Thomas–Fermi radius of about \( 15x_0 \) and a Fermi wavelength \( \lambda_F^{-1} \approx 0.2x_0 \) in the center of the trap. If we place the screen in a distance of \( z_0 = 2 \text{ cm} \) from the trap, the first minimum in the scattered intensity is only 0.3 nm away from the screen center.

For the intensity contribution due to the correlations within the gas, the typical length scale is not the radius \( R_T \) of the trap, but the much smaller Fermi wavelength \( \lambda_F \). Since the scattering angle is proportional to the inverse typical length scale, the scattered intensity due to the correlations forms a much wider light cone. The Fermi wavelength is the typical scale for all parts of the correlation function. The normal part of the pair correlation function consists of two components, namely the autocorrelation function and the Friedel oscillating part which carry opposite signs. The positive autocorrelation leads to a quasi constant intensity proportional to \( N/R^2 \), whereas the contribution of the Fermi hole with the Friedel oscillations is negative. The result is a strong suppression of the scattered intensity at small angles, reflecting the Fermi hole of the pair correlation function. While this effect could be used to detect the Fermi degeneracy in normal systems [17], the small positive contribution of the anomalous correlations also becomes significant.

To demonstrate the effect of the BCS correlations, we numerically evaluated the total intensity on a screen with distance \( z_0 = 2 \text{ cm} \) from the center of the atomic cloud. The anomalous pair correlation function was determined by a refined Simpson routine, the integrals in [15], only one of which can be performed analytically, by a Monte Carlo method. We evaluated the pair correlation function at 200 million coordinate pairs \((r, r')\) within the trap. The result is shown in figure 2, where the scattered intensity from a normal fluid and a superfluid gas of \(^6\text{Li} \) atoms are compared. For small distances \( R\perp \) from the center of the screen the superfluid phase transition significantly rises the intensity. The inset shows the ‘Fermi hole’, the drastic reduction of the observed intensity of the fermionic gas in comparison with the intensity scattered from an ideal gas of atoms, where just the autocorrelation function contributes. The typical error bars on the curves as determined by the Monte Carlo method were below 5% for the normal part and below 10% for the anomalous part.

As is shown in figure 3 the measured intensity of a normal fluid Fermi gas drops by almost 90% in comparison with the ideal gas at zero temperature. This value for the normal fluid
Fig. 2. – The total scattered intensity distribution in arbitrary units with the distance $R_\perp$ in mm from the center of the observation screen. The dashed line denotes the normal fluid state, the solid line the superfluid state. The inset also shows the intensity scattered from an ideal classical gas.

gas, however, is raised by almost 40% by the superfluid transition at small scattering angles, reflecting the softening of the Fermi hole by the anomalous correlations as in eq. (10). The peaks that occur within this graph result from side maxima of the central coherent scattering.

Fig. 3. – The ratio of the measured intensities for different states with the distance $R_\perp$ in mm from the center of the screen. The dashed line denotes the ratio of normal fluid fermionic gas to an ideal classical gas, the solid line the ratio of superfluid fermionic gas to the normal fluid gas.
peak, which for our system is about seven orders of magnitude stronger than the typical intensity caused by the correlations. Although the rise in the intensity will be smaller at finite temperatures, it should still be measurable. It is remarkable how the anomalous correlations qualitatively change the behaviour of the scattered intensity: at a fixed position one would first observe a drop in the intensity with falling temperature caused by Fermi statistics and below $T_c$ a subsequent rise.

Very recently, the suggestion to detect a BCS transition via off-resonant light scattering has also been made by Zhang et al. [12]. They found that the scattered light cone widens from an angle of order $\lambda/R$ in the normal state to an angle of order $\lambda/F$ in the presence of anomalous correlations. However in this work the normal part $g^N(x,y)$ of the pair correlation function was neglected and the authors assumed $R \approx R_\perp$ to perform the integration over the $z$-coordinate in equations (14) and (15). Therefore the cancellation between the autocorrelation and the normal part of $g(x,y)$ which is responsible for the Fermi hole and its subsequent softening by the BCS correlations is not seen in their results.

In conclusion we have performed a quantitative study of the possibility to detect a superfluid transition within a fermionic gas, e.g. $^6\text{Li}$, by measuring the intensity of off-resonant light scattered from the atomic trap. The intensity outside the central coherent scattering cone is dominated by the contributions of the pair correlation function of the system. The pair correlation function of a superfluid gas contains an anomalous part, which rises the observed intensity by as much as 40% compared to the degenerate Fermi gas, thus providing a clear signature for the onset of superfluid correlations.

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