Density and spin response functions in ultracold fermionic atom gases

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We propose a new method of detecting the onset of superfluidity in a two-component ultracold fermionic gas of atoms governed by an attractive short-range interaction. By studying the two-body correlation functions we find that a measurement of the momentum distribution of the density and spin response functions allows one to access separately the normal and anomalous densities. The change in sign at low momentum transfer of the density response function signals the transition between a BEC and a BCS regime, characterized by small and large pairs, respectively. This change in sign of the density response function represents an unambiguous signature of the BEC to BCS crossover. Also, we predict spin rotational symmetry-breaking in this system.

PACS numbers: 03.75.Hh,03.75.Ss,05.30.Fk

The BEC-to-BCS crossover has drawn renewed interest in recent years due to experimental progress in atom trap systems. Several groups achieved a Bose-Einstein condensate (BEC) in which the fermions form non-overlapping (Shafroth) pairs in a two-component Fermi gas. Despite considerable effort, much work is still needed to understand the other limit in which the pairs are large, and the pairing occurs in momentum space, similarly to the Bardeen-Cooper-Schrieffer (BCS) state of superconductivity in normal metals. Questions still remain regarding whether or not the system is superfluid when passing through the crossover with temperatures of the order of twenty percent of the Fermi temperature. The appropriate characterization of the system is still open to debate. Recently, several groups have claimed to have reached the superfluid state on the negative scattering length side of the Feshbach resonance. Despite evidence of fermionic pairing, these claims are still subject to intense discussions as no definitive proof of superfluidity is available yet.

Viverit et al. have suggested recently that the shape of the atomic momentum distribution at low temperatures is very sensitive to the sign and size of the scattering length. Altman et al. have proposed to utilize density-density correlations in the image of an expanding gas cloud to probe complex many-body states of trapped ultracold atoms. Also, Bruun and Baym showed that scattered light from a fermionic gas would exhibit a large maximum below the superfluid critical temperature and therefore it can be used to detect the superfluid transition. However it is not clear how this behavior changes close to the crossover, where the actual experiments are performed.

In this paper we propose a new diagnostic method for fermionic atomic gas condensates. By studying the zero-temperature evolution of the density and spin response functions, as a function of the scattering length of the interaction, we show that the density response function changes sign across the BEC to BCS crossover and that this change can be used to experimentally distinguish the BEC from the BCS state of the system.

Our model system consists of fermionic atoms in two hyperfine states interacting via a finite-range attractive interaction. Based on a variational approach, we also derive a sum-rule satisfied by the spin-spin correlation function at \( q = 0 \). We find that the density and spin response functions are given by the sum and the difference of independent contributions arising from the normal and anomalous density, respectively. By measuring the momentum distribution of the two response functions it is possible to infer separately the normal and anomalous densities. Finally, we predict symmetry breaking of the spin-rotation invariance. This prediction is characteristic to our model and, therefore, provides an experimental check for its applicability to real systems.

We begin by considering the two-body Hamiltonian

\[
H = \epsilon_{ki} a_{ki}^\dagger a_{ki} + \frac{1}{2} V_{q,lm,nj} a_{km}^\dagger a_{li}^\dagger a_{ip} a_{jq} a_{k+q,n},
\]

where \( \{a_{ki}, a_{ki}^\dagger\} \) are the particle creation and annihilation operators corresponding to single-particle states of linear momentum \( k \) and fermion type \( i \). The atomic levels, which we associate with the fermion types, are eigenstates of the Hamiltonian of an ion (with integer nuclear spin \( I \)) interacting with an electron (spin \( s = \frac{1}{2} \))

\[
\hat{H}_{\text{atom}} = k.e. + A \vec{s} \cdot \vec{I} + B \cdot (2 \mu_e \vec{s} - \mu_n \vec{I}),
\]

where \( A \) denotes the strength of the hyperfine interaction and \( B \) is the magnetic field, while \( \mu_e \) and \( \mu_n \) denote the electron and nuclear magnetic moments, respectively. We introduce the total angular momentum, \( \vec{F} = \vec{I} + \vec{s} \). The total angular momentum projection, \( M_F \), is the only good quantum number at finite \( B \). The atomic spectra considered in our model are depicted in Fig.

In the Hartree-Fock-Bogoliubov (HFB) formalism, one first introduces the quasi-particle creation and annihilat-
FIG. 1: Atomic states involved in the Feshbach resonance at small magnetic field, $B$, for (a) $^6\text{Li}$ and (b) $^{40}\text{K}$. The hyperfine couplings between states allowed by the selection rules are represented by dotted lines. In $^6\text{Li}$, the bound state is formed from the $F = 3/2$ states while, in $^{40}\text{K}$, it is formed from $|\frac{7}{2} - \frac{7}{2}\rangle$ and the lowest eigenstate $|\frac{7}{2} - \frac{9}{2}\rangle$.

The ground-state ansatz (3) provides a smooth interpolation between the BCS and the BEC regimes. We have recently [12] used this model to study the properties of the BEC-BCS crossover, for a short- (but finite) range and attractive interaction. In the dilute limit the model is equivalent to the zero-range (contact) interaction Hamiltonian, initially discussed by Leggett [13].

The study presented in Ref. [12] was carried out by modifying the scattering length of the interaction, while keeping the density and range of the interaction fixed. Figure 2 illustrates the momentum distributions of the normal and anomalous densities. The mean total particle-density of the system, $\rho_0$, is given by

$$\rho_0 = \langle \Phi | \hat{N} | \Phi \rangle = 2 \int \frac{d^3k}{(2\pi)^3} \rho_k. \quad (11)$$

The ground-state properties are described by the normal and anomalous densities defined as

$$\rho_k = \langle \Phi | \hat{a}_{k,\uparrow} \hat{a}_{k,\uparrow} | \Phi \rangle = |v_k|^2, \quad (9)$$

$$\kappa_k = \langle \Phi | \hat{a}_{-k,\downarrow} \hat{a}_{k,\downarrow} | \Phi \rangle = v_k^* u_k, \quad (10)$$

TABLE I: Parameters entering the modified Pauli matrices.

| Atom | a   | b   | c   | d   | $(b^2 - a^2)$ | $(d^2 - c^2)$ | bc |
|------|-----|-----|-----|-----|--------------|--------------|----|
| $^6\text{Li}$ | $\frac{1}{\sqrt{2}}$ | $\frac{1}{\sqrt{2}}$ | $\frac{1}{\sqrt{2}}$ | $\frac{1}{\sqrt{2}}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | 1  |
| $^{40}\text{K}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | 0  |

$[B \to \infty]$
where $\rho(\mathbf{r})$ and $S_\mu(\mathbf{r})$ denote the particle- and spin-density operators

$$\rho(\mathbf{r}) = \sum_{ij} a_i^\dagger \langle i | \delta(\mathbf{r} - \mathbf{r}_1) | j \rangle a_j,$$

$$S_\mu(\mathbf{r}) = \frac{1}{2} \sum_{ij} a_i^\dagger \langle i | \sigma_\mu \delta(\mathbf{r} - \mathbf{r}_1) | j \rangle a_j.$$

(14)

Here, $\sigma_\mu$ denote the Pauli matrices. Since the single-particle states are plane waves, i.e. $|i\rangle = e^{i\mathbf{k}_i \cdot \mathbf{r}} |\chi_i\rangle$, where $\chi$ denotes the $(|\uparrow\rangle, |\downarrow\rangle)$ spinors, then we can calculate the particle-density matrix element as

$$\langle i | \delta(\mathbf{r} - \mathbf{r}_1) | j \rangle = \delta_{ij} e^{i(\mathbf{k}_j - \mathbf{k}_i) \cdot \mathbf{r}},$$

(15)

and the spin-density matrix element as

$$\langle i | \sigma_\mu \delta(\mathbf{r} - \mathbf{r}_1) | j \rangle = \langle \chi_i | \sigma_\mu | \chi_j \rangle e^{i(\mathbf{k}_j - \mathbf{k}_i) \cdot \mathbf{r}}.$$  

(16)

The density response function in Eq. (15) is a scalar, while the spin density response function in Eq. (16) is a tensor. For the one-channel model the spin-response tensor is diagonal, and, provided that the Hamiltonian and the total spin operator commute, the diagonal components are equal. Then, the density and spin response functions correspond to the sum and difference of separate normal and anomalous density contributions, respectively. The nonlocal response functions can be written as

$$S_\rho(q) = \mathcal{I}_\rho(q) - \mathcal{I}_\rho(q),$$

$$S_\sigma(q) = \frac{1}{4} \left[ \mathcal{I}_\rho(q) + \mathcal{I}_\rho(q) \right].$$

(17)

Equations (18) and (19) represent a general result for the HFB mean-field approximation of the ground-state of the multi-level Hamiltonian $H$. For the one-channel model, and disregarding for now the hyperfine nature of the atomic levels involved (similarly to the case of an electron gas), the normal and anomalous density contributions to the response functions are:

$$\mathcal{I}_\rho(q) = \frac{2}{\pi^2 \rho_0} \int_0^\infty d\xi \xi^2 j_0(\xi q) \left[ \int_0^\infty dk k^2 \rho_k j_0(\xi k) \right]^2,$$

$$\mathcal{I}_\sigma(q) = \frac{2}{\pi^3 \rho_0} \int_0^\infty d\xi \xi^2 j_0(\xi q) \left[ \int_0^\infty dk k^2 \kappa_k j_0(\xi k) \right]^2.$$

(20)

The response functions $S_\rho(q)$ and $S_\sigma(q)$ are shown in Fig. 3. The density response function, $S_\rho(q)$, changes sign at low momentum, as the bound state disappears, while the spin response function, $S_\sigma(q)$, changes smoothly from the BEC to the BCS regime. In the BCS limit, the condensate wave function, $\kappa_k$, appears in a very narrow region around the Fermi momentum (see Fig. 2). Since the width of this distribution tends to zero in the limit $a_0 \to 0$, so does the anomalous density contribution, $\mathcal{I}_\rho(q)$. In turn, the density and spin response functions will be equal in this limit.

The mean-field approach shows that a measurement of the density response function is a signature of the BEC-BCS crossover. In the dilute limit, the crossover coincides with the singularity in the scattering length, which in turn corresponds to the change in sign of the density response function. Figure 3 (top) shows the dependence of $\mathcal{I}_\rho(q)$ and $\mathcal{I}_\rho(q)$, for $q = 0$, as a function of the scattering length $a_0$ at fixed density $\rho_0$ ($k_F \rho \approx 0.37$). The corresponding density response function $S_\rho(0)$ is depicted in Fig. 3 (bottom). The density response function changes

FIG. 2: (Color online) Momentum distribution of the normal and anomalous densities, as a function of the scattering length, at fixed system density, $\rho_0$ ($k_F \rho \approx 0.37$). Inset shows the density of states. We use the notation $\eta = (a_0 k_F)^{-1}$.

FIG. 3: (Color online) The density and spin instantaneous response function for an electron gas, as a function of the scattering lengths, at fixed density, $\rho_0$. 

FIG. 4 (top). The density response function changes
sign between the BCS and the BEC limits.

The one-channel model predicts that the spin response function at zero momentum transfer, $S_\sigma(q = 0)$, is in fact a sum rule, i.e.

$$S_\sigma(0) = -\frac{1}{4\pi^2\rho_0} \int_0^\infty dk \ k^2 (\kappa_k^2 + \rho_k^2) = -\frac{1}{4}, \quad (22)$$

or $I_\sigma(0) + \kappa_\sigma(0) = 1$ is independent of $\eta = (a_0 k_F)^{-1}$, as shown in Fig. 4 (top). The above is obtained by using the definitions (9) and (10), together with the normalization condition, Eq. 14.

We now consider the modification of the electron gas results, due to the hyperfine nature of the interacting atomic levels. We find the spin response function is proportional to the “weighted” difference of the normal and anomalous density contributions derived earlier, $I_\sigma(q)$ and $\kappa_\sigma(q)$. The weighting factors depend on the atom specie in the system, and the atomic levels involved in the interaction. Since the spin response function is only sensitive to the electron spin operator, then in order to find the modification of the spin response function, we need to calculate the matrix elements $\langle \chi_i | \sigma_j | \chi_j \rangle$ in Eq. 14. The parameters entering the modified Pauli matrices are

$$\sigma_0 \rightarrow \begin{pmatrix} b^2 - a^2 & 0 & 0 \\ 0 & d^2 - c^2 & 0 \end{pmatrix}, \quad \sigma_\pm \rightarrow bc \sigma_\pm, \quad (23)$$

and limiting values as a function of the magnetic field, $B$, are listed in Table I. We note that in the large field limit, the spin response in a $^6$Li fermionic atom gas has opposite sign as compared to the case of a $^{40}$K fermionic atom gas. Irrespective of the actual B value, we obtain that for a fermionic atom gas, the rotational symmetry of the spin response function is broken. This symmetry-breaking effect is a prediction of our model, and arises as a consequence of the fact that our effective interaction involves a restricted set of atomic levels.

In conclusion, in this paper, we have shown that much information about the crossover regime can be gained by experimentally studying the density and spin response functions. Within the framework of the mean-field results, we show that the normal and anomalous densities can be accessed from the momentum distribution of the response functions. The spin response function changes smoothly across the crossover, while the density response function changes sign, and thus represents a signature of the crossover. The spin response at zero-momentum transfer satisfies a sum rule, and is sensitive to the interaction. When taking into account the hyperfine structure of the interacting levels, our model predicts that the rotational invariance of the spin response, normally associated with an electron gas subject to a spin-independent interaction, is broken.

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