Establishing the Presence of Coherence in Atomic Fermi Superfluids: Spin-Flip and Spin-Preserving Bragg Scattering at Finite Temperatures

Hao Guo 1, Chih-Chun Chien2 and K. Levin1

1James Franck Institute and Department of Physics, University of Chicago, Chicago, Illinois 60637, USA and
2Theoretical Division, Los Alamos National Laboratory, MS B213, Los Alamos, NM 87545, USA

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We show how the difference between the finite temperature $T$ structure factors, called $S_-$, associated with spin and density, can be used as a indication of superfluidity in ultracold Fermi gases. This observation can be exploited in two photon Bragg scattering experiments on gases which undergo BCS- Bose Einstein condensation crossover. Essential to our calculations is a proper incorporation of spin and particle number conservation laws which lead to compatibility at general $T$ with two $f$-sum rules. Because it is applicable to general scattering lengths, a measurement of $S_-$ can be a useful, direct approach for establishing where superfluidity occurs.

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One of the most intriguing aspects of the ultracold Fermi gases in the strongly interacting, attractive regime is the difficulty they pose for establishing superfluidity. The absence of indications from the density profiles, along with the presence of a normal state excitation gap are all responsible for this difficulty. Most experiments [1–4] which determine whether a state is superfluid or not, make use of a fast sweep of the magnetic field into the low field Bose Einstein condensation (BEC) limit, where the superfluid signatures are more straightforward. Thermodynamical properties do not establish whether the phase is ordered or not, although they can determine where $T_c$ lies [5, 6]. It would be particularly useful then to find a neutral fluid counterpart to the Meissner experiment for Fermi gases with attractive interactions. More specifically, we want to find a property which reflects the superfluid order parameter such that it is non-zero below $T_c$ and vanishes above. Of particular interest is Bragg spectroscopy [7] which is capable of detecting true superfluid coherence. This is to be contrasted with radio frequency spectroscopy [8] which is most suited for establishing pairing.

It is the purpose of this paper to address this goal by presenting a theory of the spin preserving and spin flip dynamical responses at general temperatures in a homogenous gas. Both of these can, in principle, be measured via two photon Bragg scattering. Our emphasis here is on the contrasting physics of spin density and particle density which we demonstrate allows a separation of coherent order from pairing effects. While we focus on unitary gases, we also present results associated with both the BCS and the BEC sides of resonance. Indeed, there has been considerable theoretical interest in combined studies of spin and particle density Bragg scattering at zero temperature in BCS-BEC crossover theory [6, 10] as well as of spin-flip Bragg experiments above $T_c$ [11].

Two aspects are essential to a proper theory of Bragg scattering. (i) At all temperatures the identities based on conservation laws for particle number and spin need to be satisfied:

$$\lim_{q \rightarrow 0} S_{C,S}(\omega, q) = 0,$$

where $S_{C,S}(\omega, q)$ are the dynamical structure factors for the particle density (labelled $C$) and the spin (labelled $S$). Here $n_F$ is the total density of particles. The first equation is the well known $f$-sum rule in the form associated with the generalized BCS Hamiltonian. In past work [11] sum rules were found to be difficult to implement in the presence of pairing correlations. (ii) Below $T_c$, collective mode physics in the charge channel is responsible for Eq. (2), not Pauli blocking as is sometimes claimed; this ensures current conservation and restores the $U(1)$ gauge symmetry.

We define

$$S_\pm(\omega, q) = \frac{1}{2}[S_C(\omega, q) \pm S_S(\omega, q)].$$

From Eq. (1) an important additional sum rule then follows

$$\int_{-\infty}^{\infty} d\omega S_-(\omega, q) = 0.$$  (4)

The quantity $S_-(\omega, q)$ represents a measure of “spin density and particle density separation”. In the literature [9] the quantity $S_{\perp} \equiv 2\langle \rho(\mathbf{r})\rho_i(\mathbf{r}) \rangle$ is defined in the same way as $S_-$. Importantly, $S_{\perp}$ has been argued [9, 12] to be proportional to the density density correlation function $\langle \rho(\mathbf{r})\rho_i(\mathbf{r}) \rangle$. The sum rule of Eq. (4) indicates that $S_{\perp}$ times frequency integrates to zero. In strict BCS theory this sum rule is satisfied because $S_-(\omega, q)$ (or equivalently $S_{\perp}(\omega, q)$) has negative weight below $T_c$ and is identically zero above $T_c$. In this paper we show that the behavior found in strict BCS is general. On this basis, we argue that the association of the density-density correlation function (with opposite spin) and the quantity $S_{\perp}(\omega, q)$ (or equivalently $S_-(\omega, q)$) is very problematic. Collective mode effects are, in part, the reason that naive linear response theory (relating $\langle \rho(\mathbf{r})\rho_i(\mathbf{r}) \rangle$ to $S_{\perp}$) fails below $T_c$.

The theoretical approach used here is based on the BCS-Leggett ground state wavefunction, which has been shown [9]...
to give a reasonable description of the $T = 0$ spin and density dynamical structure factors as computed using quantum Monte Carlo simulations. Here we generalize this treatment of BCS-BEC crossover to finite $T$ and must choose the appropriate diagram set to respect the conservation laws in Eqs. (1) and (2). The present approach is most well suited to address these sensitive issues which arise in gauge invariant electrodynamics; here in contrast to other crossover schemes [13] the superfluid density is well behaved and monotonic in $T$. We build on the analysis outlined in Ref. [14] which focused principally on collective mode effects. In this extension of the ground state to finite $T$, the pairing gap $\Delta(T)$ has two contributions associated with condensed (sc) and non-condensed (pg) pairs such that $\Delta^2 = \Delta_{\text{sc}}^2 + \Delta_{\text{pg}}^2$. The latter vanishes at $T = 0$ and the former vanishes at $T_c$ and above.

For spin-preserving and spin flip Bragg processes [15] the external field Hamiltonian contains contributions of the form $\int d^3r [\lambda^{C,S}_{(\sigma')} \Psi_{(\sigma')} \Psi_{(\sigma)} + \text{h.c.}]$ where $\lambda^{C}_{(\sigma)} \propto \delta_{\sigma \sigma'}$ and $\lambda^{S}_{(\sigma)} \propto \delta_{\sigma \sigma'}$. Here $\Psi_{(\sigma)}$ is the fermionic creation (annihilation) operator, $\sigma = \uparrow, \downarrow$ and $\sigma' = -\sigma$. While there would seem to be a similarity in these two channels we stress that there is also a physical difference. In the superfluid phase, due to coherent singlet pairing, the response functions of spin and particle densities are different, whereas one may anticipate that they are the same in the normal phase. Indeed, linear response theory based on the above Hamiltonian is incomplete; it will not lead to a consistent treatment of the density preserving response, because it ignores collective mode effects below $T_c$. For the unperturbed Hamiltonian of the BCS type, and for singlet pairing, spin is conserved. However, because the spin degrees of freedom are not associated with a spontaneous symmetry breaking, they do not lead to collective phase modes upon condensation.

In the density channel, linear response theory is more complex; we introduce a four-vector formalism with “electromagnetic” (EM) field $A_\mu$ where $\mu = 0, 1, 2, 3$. The induced EM current $J_\mu$ is given by $J_\mu(Q) = K^{\mu\nu} A_\nu(Q)$, where, $Q = (\omega, \mathbf{q})$, is the four-momentum and the EM response kernel, $K^{\mu\nu}$, can be written as $K^{\mu\nu}(Q) = K_0^{\mu\nu}(Q) + \delta K^{\mu\nu}(Q)$, where $K^{\mu\nu}$ is the correction due to collective mode effects [14]. Here $\delta K^{\mu\nu}$, which is essential for charge conservation ($q_\mu K^{\mu\nu}(Q) = 0$), has a vanishing denominator [14] associated with the order parameter collective mode dispersion. In this letter, we are interested in the (0)-component of the EM kernel, which corresponds to the gauge invariant density-density response function $\chi_{\rho\rho}(\omega, Q) \equiv \chi_{00}(\omega, Q)$. This, in turn, is related to the dynamic structure factor in the density channel, given by $S_C(\omega, Q) = -\frac{1}{2} \coth(\frac{\omega}{2}) \text{Im} \chi_{00}(\omega, Q)$, where $\chi_{\rho\rho}(\omega, Q)$ represents the properly gauge invariant form of the density-density response function. In a similar way, the dynamic spin structure factor is $S_S(\omega, Q) = -\frac{1}{2} \coth(\frac{\omega}{2}) \text{Im} \chi_{SS}(\omega, Q)$, where $\chi_{SS}(\omega, Q)$ is the spin-spin response function.

Now we turn to finite temperatures where there is little prior work addressing Bragg scattering in the crossover scenario. Charge conservation and gauge invariance which can be explicitly shown to hold at the BCS level must be respected [14] even in the presence of pairing correlations. The best way to insure these is to establish that the $f$-sum rules Eq. (1) and the related Eq. (2) are satisfied [14]. For our BCS-Leggett ground state, extended to $T \neq 0$, the diagrammatic corrections to the EM vertex have been discussed [14] and are indicated in Fig. 1. There are two types of contributions shown as Maki-Thompson (MT) and Aslamazov-Larkin (AL$_{1,2}$) diagrams.

The “bare” part of the EM response kernel is given by $K_0^{\mu\nu}(Q) = -\frac{Q_\mu Q_\nu}{m^2} g^{\mu\nu}(1 - g^{\mu\nu}) = 2 \sum_K \lambda^K(K, K - Q) G(K) G(K - Q) \Lambda^K(K, K - Q)$, (5)

where the bare and full EM vertex are $\lambda^K(K, K + Q) = (1, \frac{1}{m}(k - q))$ and $\Lambda^K = \lambda^K + \delta \Lambda_{\omega m} + \delta \Lambda_{pg}$ respectively. Here $m$ is the particle mass and $g^{\mu\nu}$ is the metric tensor. Note that the full vertex $\Lambda$ does not include collective mode physics and, thus, is not gauge invariant below $T_c$, while the vertex $\Lambda'$ contained in the AL$_2$ diagram is gauge invariant. Importantly, consistency with the Ward identities will lead a cancellation [14] between the MT and AL terms $\frac{1}{2} (\text{AL}_1 + \text{AL}_2) + \text{MT}_C = 0$. Throughout we use the superscript “C” to refer to the density response and the counterpart “S” for the spin counterpart.

After imposing the Ward identities [14], the dynamical
structure factor for particle density can be written as the sum of five terms

\[ S_C = S_{C0} + S_{MT_{\parallel}} + S_{MT_{\perp}} + S_{AL} + S_{coll}, \]  

where the first term on the right-hand-side denotes the "bare" term from \( K_{00}^{(0)} \). The remaining terms denote the corrections from the MT, and two AL diagrams and from the collective modes.

In the spin channel, the spin-“magnetic field” interaction also contains effects associated with pairing fluctuations, but there is a significant difference. Here the AL diagrams are not included. This assertion can be verified by establishing numerical consistency with the \( f \)-sum rule \([1]\). It is also, then, consistent with the equality in Eq. (2). As a result, the full vertex is given by \( \Lambda_S = \lambda_S + \delta \Lambda_{MT_{\parallel}} + \delta \Lambda_{MT_{\perp}} \). Here the bare spin-magnetic field interaction vertex is \( \lambda_S(P, P + Q) = 1 \). Diagrammatically these contributions are represented by the first two terms on the right hand side in Fig. 1. The full spin response function is given by \( \chi_{SS}(Q) = \)

\[ 2 \sum_K \lambda_S(K, K - Q)G(K)G(K - Q)\Lambda_S(K, K - Q). \]  

We arrive at a final compact expression for the spin structure factor

\[ S_S = S_{S0} + S_{MT_{\parallel}} + S_{MT_{\perp}}. \]  

We now evaluate \( S_-(\omega, q) \). It can be shown that \( S_{C0} = S_{S0} \). Moreover, the MT terms in the spin and density channel enter with reversed signs, as has been noted previously \([10]\): \( S_{MT_{\parallel}} = -S_{MT_{\parallel}} \) and \( S_{MT_{\perp}} = -S_{MT_{\perp}} \). Together with the cancellation between MT and AL terms, we arrive at a very general form for \( S_- \), defined in Eq. (5).

\[ S_- = S_{MT_{\parallel}} + \frac{1}{2} S_{coll}. \]  

Importantly, \( S_-(\omega, q) \) depends only on the order parameter; it vanishes above \( T_c \), as is trivially consistent with the sum rule in Eq. (4). For the strict BCS case, where the same behavior obtains, one can clearly see that this is not a consequence of

| \( q/k_F \) | \( f_{\omega M}^{(0)} \) | \( f_{\omega M}^{(1)} \) | \( f_{\omega M}^{(2)} \) | \( f_{\omega M}^{(3)} \) |
|---|---|---|---|---|
| -1.0 | 0.06 | 1.000 | 0.991 | \( \sim 20 \) |
| -0.5 | 0.12 | 0.999 | 0.999 | |
| 0.0 | 0.12 | 0.976 | 0.941 | \( \sim 100 \) |
| 1.0 | 0.25 | 0.910 | 0.910 | |

Table I: \( f \)-sum rule tests for density and spin structure factors in BCS-BEC crossover. \( \omega_M \) is the maximum frequency. The expected value is 1.0 in units of \( n_F k_F / 2 \).

the vanishing of the gap, but rather of true phase coherence. Above \( T_c \) the same diagrams leading to the vanishing of the superfluid density \([14]\) are responsible for the vanishing of \( S_- \).

This discussion has been general; now we substitute our specific form for the self energy \([14]\) to obtain

\[ K_{00}^{(0)}(\omega, q) \text{ or } \chi_{SS}(\omega, q) = \sum_{\mathbf{p}} \left[ (1 - f_+ - f_-) \times \right. \]

\[ \frac{E_+ + E_-}{E_+ - E_-} \left( \frac{E_+ - E_-}{\omega^2 - (E_+ + E_-)^2} + \frac{E_+ - E_-}{\omega^2 - (E_+ - E_-)^2} \right) \]  

\[ \left. \times \left( \frac{E_+ - E_-}{\omega^2 - (E_+ + E_-)^2} + \frac{E_+ - E_-}{\omega^2 - (E_+ - E_-)^2} \right) \right]. \]  

Here \( E_{\pm} = E_{\mathbf{p} \pm q/2}, f_{\pm} = f(E_{\pm}), \) and \( \omega \) implicitly has a small imaginary part. The factor "sgn" is 1 and \(-1\) in the density and spin channels respectively. Note that as a result of these sign changes in Eq. (10), the dynamical correlations in the spin channel depend only on the square of the pairing gap \( \Delta \) which involves the sum of the squares of \( \Delta_{pq} \) and \( \Delta_{sc} \). This is very different from the particle density channel which reflects the distinction between condensed (sc) and non-condensed (pg) pair contributions.

We now establish that the sum rules (Eq. 11) are satisfied along with Eq. (2). For illustration purposes, we choose a fixed momentum transfer \( q = 0.5k_F \), and list the results of our sum rule checks for various scattering lengths \( k_F a \) and two different temperatures (above and below \( T_c \)) in Table II. Both sum rules are satisfied to within 10% or better. In the table \( \omega_M \) is the maximal frequency up to which we integrate in order to satisfy the sum rules. We found that both structure factors approach zero. On the BCS side, the structure factors decay extremely rapidly so that \( \omega_M \) need not be large, but on the BEC side of resonance, they exhibit a long and slowly
decaying tail. The characteristic size of this upper bound is of interest experimentally in measurements of the structure factor (which reflect the frequency integrated form of \(S(\omega, q)\)) such as in Ref. [12]. We have also verified that the \(f\)-sum rule holds for large momentum transfers; at unitarity where our studies are most complete, the errors are smaller than 5%.

Fig. 2 presents a plot of the two static structure factors \(S_+(q)/2\) and \(S_-(q)\) as a function the momentum transfer at unitarity and for two different temperatures below and above \(T_c\). The large \(q\) behavior at the lower \(T\) is consistent with the \(T = 0\) results in Ref. [9]. At small \(q\), all structure factors approach zero as required by Eq. (9). Fig. 2 is a central figure of this paper. Here we plot \(S_-(q)\) as a function of temperature, which one can see behaves like an order parameter. The same result can be obtained for any fixed \(q\) and \(\omega\) and reflects the behavior implicit in Eq. (9). That is, the difference between the density and spin channels arises only in the presence of a condensate. This behavior is also found in strict BCS theory as well as for any \(k_F\). The vanishing of \(S_-\) signals the vanishing of condensation. It should establish if an unknown Fermi gas is in the superfluid or normal phase.

Fig. 3 shows the particle density (solid lines) and spin response (dashed lines) in units of \(n_F/2e_F\) as a function of \(\omega/\epsilon_F\). We show temperatures both below and above \(T_c\) for a fixed momentum transfer \(q = 0.5k_F\) and for various \(k_F\). Above \(T_c\), the magnetic and density response contributions coincide. Below \(T_c\), one sees from Fig. 3 that \(S_+(q, \omega)\) has two main features, a collective mode peak, and a continuum of quasiparticle excitations which appears for \(\omega > 2\Delta\), associated with the breaking of Cooper pairs induced by the perturbation. The “collective” peak is broadened somewhat due to coupling to the continuum. As the system evolves from the BCS to the BEC regime (where the pairs are more difficult to break), this “collective” peak contains increasingly more of the total spectral weight contained in the \(f\)-sum rule. Above \(T_c\), the spectral weight in the former “collective” peak must be redistributed, leading to an increased contribution in the continuum and to a new low frequency peak which is associated with thermally broken pairs. This peak appears at unitarity and on the BCS side of resonance for the considered range of temperatures. At a more formal level it arises from the contributions from the AL diagrams when \(\mu > \frac{1}{m^2} \left(\frac{q}{2}\right)^2\) above \(T_c\). These two continua nearly merge in the BCS regime in Fig. 3(a); they are separated for the unitary and BEC cases.

Turning now to the spin structure factor at low \(T\) (denoted by dashed lines in Fig. 3), it can be seen that there is no collective physics. The entire spectral weight of the \(f\)-sum rule is associated with the continuum, and this, in turn, only appears when \(\omega > 2\Delta\) where the energy transfer is large enough to break pairs. Just as for the particle density response, we see that the low frequency spectral weight is highly suppressed. In the BEC regime, in Fig. 3(d), the spectral weight does not change significantly with \(T\), since the temperatures considered were not sufficient to break pairs. This behavior is consistent with that found earlier [11] on the BEC side of resonances. There is also a small low frequency peak, which gives a tiny contribution to the \(f\)-sum rule.

In this paper we proposed a methodology for establishing phase coherence in neutral superfluids. This has been a long standing issue with one of the earliest such proposals based on noise correlations [13], although this has proved difficult to implement away from \(T = 0\). Here, by contrast we propose two photon Bragg experiments at \(T \neq 0\) which measure the difference between the dynamical responses associated with the particle and spin density, called \(S_-(\omega, q)\) (or [12] \(S_{1\gamma}(\omega, q)/2\). The qualitative behavior shown in Figure 2b, also obtains for \(|S_-(\omega, q)|\) for all \(q, \omega\). This signature of phase coherent order, unlike others in the past based on Bragg scattering, requires looking at a single \(q, \omega, T\). It should also apply to other crossover schemes which satisfy the conservation laws, to trapped gases and to optical lattices (at least) for frequencies below those of the band gaps.

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