Static structure factor of a strongly correlated Fermi gas at large momenta

H. Hu\textsuperscript{1,2(a)}, X.-J. Liu\textsuperscript{1} and P. D. Drummond\textsuperscript{1}

\textsuperscript{1} ARC Centre of Excellence for Quantum-Atom Optics, Centre for Atom Optics and Ultrafast Spectroscopy, Swinburne University of Technology - Melbourne 3122, Australia
\textsuperscript{2} Department of Physics, Renmin University of China - Beijing 100872, China

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Abstract – We theoretically investigate the static structure factor of an interacting Fermi gas near the BEC-BCS crossover at large momenta. Due to short-range two-body interactions, we show that the structure factor of unlike spin correlations \( S_{\uparrow \downarrow}(q) \) falls off as \( 1/q \) in a universal scaling region with large momentum \( \hbar q \) and large scattering length. The scaling coefficient is determined by the celebrated Tan’s contact parameter, which links the short-range behavior of many-body systems to their universal thermodynamic properties. By implementing this structure-factor Tan relation together with the random-phase approximation and the virial expansion theory in various limiting cases, we show how to calculate \( S_{\uparrow \downarrow}(q) \) at zero and finite temperatures for arbitrary interaction strengths, at momentum transfer higher than the Fermi momentum. Our results provide a way to experimentally confirm one of the Tan relations and to accurately measure the value of contact parameter.

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Strongly interacting fermions are an important feature of many physical systems in condensed-matter physics, nuclear physics and astrophysics. The recent achievements of trapping and cooling ultracold fermionic atoms have made them significant in atomic physics as well [1]. With the unprecedented controllability of interactions and geometries [1], these atomic systems are prototypes of many important theoretical models. The strength of the interactions is governed by a single (i.e., \( s \)-wave) two-body scattering length, and can be tuned by means of Feshbach resonances, allowing for a systematic exploration of the crossover from a weakly coupling BCS superfluid to a Bose-Einstein condensate (BEC) of tightly bound molecules. Ultracold atoms therefore provide a new platform for investigating the intriguing many-body properties of fermions. A rich variety of theoretical predictions has emerged, many of which await verification. Theoretical challenges arise especially when the scattering length \( a \) is comparable to or larger than the inter-particle distance \( l \) [2]. In this strongly interacting regime, the system has universal scaling properties that depend on \( l \) only [3,4]. These universal properties, however, cannot fully be understood using conventional perturbation methods, which are reliable only for \( a \ll l \) [5,6]. \textit{Ab initio} quantum Monte Carlo (QMC) simulations are very helpful [7,8], but suffer from the Fermi sign problem in many cases. The challenging nature of strong interactions therefore makes \textit{exact} results very valuable.

In this letter, we discuss theoretically an exact relation for the large-momentum behavior of the spin-antiparallel static structure factor \( S_{\uparrow \downarrow}(q) \), showing that it has a simple universal power-law \( (1/q) \) tail. This power-law behavior was recently confirmed at Swinburne University, using \(^6\)Li atoms near a Feshbach resonance at nearly zero temperature [9]. Here, we present the theoretical details.

The relation we consider, hereafter referred to as the structure-factor Tan relation, belongs to the family of exact relations obtained by Tan in 2005 [10], which link the short-range, large-momentum, and high-frequency asymptotic behavior of many-body systems to their thermodynamic properties [10–14]. For instance, the momentum distribution and rf spectrum fall off as \( q^{-4} \) and \( \omega^{-5/2} \), respectively. All the Tan relations are related to each other by a single coefficient \( \mathcal{I} \), referred to as

\textsuperscript{(a)}E-mail: hhu@swin.edu.au

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the integrated contact density or contact. The contact measures the probability of two fermions with unlike spins being close together [15]. It also links this short-range behaviour to thermodynamics via the adiabatic relation, \( dE/d(-1/a) = \hbar^2 t/(4\pi n) \), which gives the change in the total energy \( E \) due to adiabatic changes in the scattering length. The fundamental importance of the Tan relations is due to their wide applicability: to zero or finite temperature, superfluid or normal phase, homogeneous or trapped, few-body or many-body systems.

The structure-factor Tan relation for \( S_{\uparrow\downarrow}(q) \) follows directly from the short-range behavior of the pair correlation function \( n_{\uparrow\downarrow}^{(2)}(r) \equiv \int d\mathbf{r} \langle \hat{n}_\uparrow(\mathbf{r} - r/2)\hat{n}_\downarrow(\mathbf{r} + r/2) \rangle \), which diverges as

\[
n_{\uparrow\downarrow}^{(2)}(r \to 0) \approx \frac{T}{16\pi^2} \left( \frac{1}{r^2} - \frac{2}{ar} \right).
\]

A Fourier transformation of \( n_{\uparrow\downarrow}^{(2)}(r \to 0) \) then leads to

\[
S_{\uparrow\downarrow}(q > k_F) \approx \frac{T}{4Nq} \left[ 1 - \frac{4}{\pi aq} \right] \equiv \frac{T}{Nk_F} f(q),
\]

where \( k_F \) is the Fermi wave vector and \( N \) is the total number of atoms. On the right-hand side of the above equation, we have defined \( t(q) \equiv \left| k_F/(4aq) \right| [1 - 4/(\pi aq)] \).

Equation (2) holds in a scaling region of sufficiently large \( q \) near the unitarity limit (\( a \to \pm \infty \)). It follows from the Taylor expansion of the expression agrees exactly with eq. (2), since

\[
I_{\text{BEC}}/(Nk_F) \approx \frac{4\pi}{(k_Fa)}. \]

In the opposite BCS limit of \( 1/(k_Fa) \to -\infty \), we follow a mean-field picture and treat the system as a gas of quasiparticles subjected to a (dynamical) mean-field Hamiltonian

\[
\hat{H} = \hat{H}_0 + (4\pi \hbar^2 a/m)(\delta n_\sigma + \delta n_\bar{\sigma}),
\]

where \( \hat{H}_0 \) is the free-particle Hamiltonian and \( \delta n_\sigma = \delta n_\sigma(\mathbf{r},t) \) are the space- and time-dependent density fluctuations with respect to equilibrium. Here, we consider a normal state since the result differs by an exponentially small amount from that of the BCS superfluid state. The dynamic structure factor \( S_{\sigma\bar{\sigma}}(q,\omega;T) \) may be calculated via the density response functions within a (random-phase) linear response theory [17], which are given by

\[
\chi_{\sigma\bar{\sigma}} = \chi_{\sigma\sigma}^0 + \sum_{\sigma''\bar{\sigma}''} \chi_{\sigma\sigma}^{(0)}(4\pi \hbar^2 m/a)m \chi_{\sigma''\bar{\sigma}''}^{\lambda}(qT). \]

The free response function \( \chi_{\sigma\sigma}^{(0)} \) can be written in a simple form in terms of a dimensionless function \( g(q,\lambda;T) \):

\[
g(q,\lambda;T) = \int \frac{d\omega}{2\pi} \left[ \frac{1}{\lambda} \right] \left[ \frac{m}{\hbar \omega} \right] \left[ \frac{m\omega}{\hbar q} \right] \left[ \frac{m\omega}{\hbar q} \right],
\]

with \( \bar{q} \equiv q/k_F, \lambda \equiv m\omega/(\hbar q k_F) \), and \( T = \pi T/4\). The function \( g(q,\lambda;T) \) can be found in standard textbooks [17]. In leading order in \( k_Fa \), it is straightforward to show

\[ [S_{\sigma\bar{\sigma}}(q > k_F)]_{\text{BEC}} \approx \frac{2}{qa} \arctan \left( \frac{qa}{2} \right), \]

which is essentially geometry and temperature independent. For \( qa \gg 1 \), the first two terms in the Taylor expansion of the expression agrees exactly with eq. (2), since

\[ I_{\text{BEC}}/(Nk_F) \approx \frac{4\pi}{(k_Fa)}. \]
that for a *homogeneous* Fermi gas, the static structure factor $S_{↑↓}(q) \equiv (2/N) \int d\omega S_{↑↓}(q, \omega; T)$ is given by

\[
[S_{↑↓}(q)]_{\text{BCS}} \simeq -\frac{12k_F a}{\pi^2} q \int_{-\infty}^{\infty} d\lambda \frac{\text{Re} g(\tilde{q}, \lambda; T) \text{Im} g(\tilde{q}, \lambda; T)}{1 - \exp[-2\tilde{q}\lambda/T]},
\]

This weak-coupling equation holds for arbitrary transferred momentum. We may rewrite it into the form,

\[
[S_{↑↓}(q)]_{\text{BCS}} \simeq \mathcal{I}_{\text{BCS}}/(Nk_F) [-\pi^2/(4\pi qa)] f(\tilde{q}; T)/(4q/k_F),
\]

where at $T = 0$ we have defined $f(\tilde{q}; T = 0) \equiv (9/\pi)^2 \int_0^\infty d\lambda \text{Re} g(\tilde{q}, \lambda; 0) \text{Im} g(\tilde{q}, \lambda; 0)$ and have confirmed that $\mathcal{I}_{\text{BCS}}/(Nk_F) \simeq 4(k_F a)^2/3$ [10]. At large momentum, asymptotically, $f(\tilde{q} \gg 1; T = 0) = 1 + 2/(5q^2) + O(q^{-4})$. Thus, at the leading order of interaction strengths ($\sim k_F a$), the structure factor in the BCS limit is in agreement with the Tan relation (2). We note, however, that the dominant $1/q$ tail in the strongly interacting regime (i.e., the factor 1 in the square bracket in eq. (2)) is lost. The large momentum tail comes from pairing effects and therefore cannot be captured by the random-phase approximation for linear response.

**Structure factor from an interpolation strategy.**

– The excellent agreement between the large-$q$ expansion of the weak-coupling results, eqs. (3) and (4), and the Tan relation (2) suggests that we may use the following extrapolation for the calculation of the structure factor at $q > k_F$ and at arbitrary interaction strengths:

\[
S_{↑↓} \simeq \left( \frac{\mathcal{I}}{Nk_F} \right) \times \begin{cases} 
\{k_F/(4q)[1 - 4f(q/k_F; T/T_F)/(\pi qa)]\}, & a < 0; \\
\{k_F/(2\pi qa)\arctan(qa/2)\}, & a > 0.
\end{cases}
\]

In doing so, we remove the severe requirements of $q \gtrsim k_F$ and $q \gtrsim 1/a$ for validating the Tan relation (2). In fig. 1, we show the resulting static structure factor $S_{↑↓}(q = 3k_F)$ for a homogeneous Fermi gas along the BEC-BCS crossover. We have determined the contact $\mathcal{I}$ by applying the adiabatic relation to the ground-state energy calculated from a perturbative Gaussian pair fluctuation theory [6]. In the figure, the weak coupling results in eqs. (3) and (4) are also reported respectively by the dashed and dot-dashed lines. By applying a local density approximation, we may also calculate the zero temperature structure factor of a Fermi gas in a harmonic trap with frequency $\omega_0$ and length $a_{ho} = \sqrt{\hbar/m\omega_0}$. Using the ideal Fermi temperature and vector at the trap center, $k_BT_F = (3N)^{1/3}\hbar\omega_0$ and $k_F = (24N)^{1/6}/a_{ho}$, we find that the trapped structure factor differs only slightly with the uniform one (see the black line in fig. 2).

The accuracy of the interpolation may be justified by comparing our results to QMC simulations [8], as shown in the inset for $q = 2k_F$, $3k_F$, and $5k_F$. We find a large deviation occurring at $q < k_F$ on the BEC side (not shown in the inset), where one has to take into account the correlations between different bound molecules. However, this is irrelevant to our purpose of examining large-momentum correlations. As we shall see, a further justification of our

**Fig. 1:** (Colour on-line) Zero temperature ($T = 0$) spin-antiparallel static structure factor of a homogeneous Fermi gas along the BEC-BCS crossover at $q = 3k_F$, calculated by using the interpolation strategy as described in the text (eq. (5)). The red dashed and blue dot-dashed line show the asymptotic behavior in the weak-coupling BEC (eq. (3)) and BCS (eq. (4)) regime, respectively. The inset compares our interpolation results (lines) with the QMC simulations (symbols) [8]. The excellent agreement at large momentum justifies our interpolation idea.

**Fig. 2:** (Colour on-line) Temperature dependence of spin-antiparallel static structure factor in a harmonic trap. The zero-temperature result is obtained by applying a local density approximation to the homogeneous structure factor. The inset shows a comparison of the leading virial expansion predictions (symbols, eq. (7)) with the interpolation strategy (lines, eq. (5)), where $f(\tilde{q}; T)$ is averaged over the trap. This excellent agreement therefore justifies the interpolation strategy at finite temperatures.

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We find that \( f(q, T) = \frac{q}{\sqrt{T}} \int_{-\infty}^{+\infty} u(x) \exp \left[ -\frac{(x - q)^2}{2T} \right] \, dx \),
where the function \( u(x) \equiv \int_0^\infty dt e^{-e^{-t^2} - e^{-t^2}/t} \). We find that \( f(q) \approx 1; \, T = 1 + \frac{T}{(q^2) + O(q^{-4})} \).

Quantum virial expansion at finite temperatures. We now calculate the structure factor at high temperatures for a trapped Fermi gas, by extending a previous virial expansion theory \([18–20]\). At high temperatures, the fugacity \( z \equiv \exp(\mu/k_BT) \ll 1 \) is a small controllable parameter, even in the strongly interacting limit. We may expand the thermodynamic potential \( \Omega = -k_BT \ln Z \), where \( Z = \text{Tr} [\exp(-\mathcal{H} - \mu N)/k_BT] \), in a series of powers of fugacity. By defining partition functions of clusters in the \( n \)-particle subspace, \( Q_n = \text{Tr}_n[\exp(-\mathcal{H}_n/k_BT)] \), we find that \( \Omega/k_BT = -[zQ_1 + z^2(Q_2 - Q_1^2/2) + \cdots] \). The pair correlation function \( n_{2\nu}^{(2)}(\mathbf{R}, \mathbf{r}) = \langle \langle \hat{n}_{\nu}(\mathbf{r}_1) \hat{n}_{\nu}(\mathbf{r}_2) \rangle \rangle \), which can already be obtained from the leading two-body state of a trapped Fermi gas. The fugacity is given by \( \exp(-\mathcal{H}_n/k_BT) \), and so on. However, considerable insight can already be obtained from the leading two-body contribution shown in eq. (7). At short distance, \( \psi_{\nu \alpha}(r) = (2\pi)^{3/2}/(2\nu a)^{3/2} \exp \left[ -r^2/(4\nu a^2) \right] \). Therefore, for large-momentum transfer \( q \), we find from eq. (7) that

\[
S_{\uparrow \downarrow}(q) = \frac{I_{VE}}{4Nq} \left[ 1 - \frac{4}{\pi a q} + \frac{16}{\sqrt{3\pi a^2 \hbar^2 \omega_0}} \frac{d\ln B}{dq} \right],
\]
where \( B(\beta) \equiv \sum_n \exp[-\beta(2\nu_n + 3/2)] \pi a^2 \) and

\[
I_{VE} = 4\pi x^2 \left[ \frac{1}{(e^{+\beta} - e^{-\beta})^3} \right] \equiv (e^{+\beta} - e^{-\beta})^3 \left[ \frac{1}{(e^{+\beta} - e^{-\beta})^3} \right] \equiv \frac{1}{(e^{+\beta} - e^{-\beta})^3} \left[ \frac{1}{(e^{+\beta} - e^{-\beta})^3} \right] \equiv \frac{1}{(e^{+\beta} - e^{-\beta})^3} \left[ \frac{1}{(e^{+\beta} - e^{-\beta})^3} \right].
\]

In fig. 2, we present the numerical results of the leading virial expansion for the static structure factor \( (q = 3k_F) \) of a trapped Fermi gas. The fugacity \( z \) is determined by the number equation, \( N = -\partial \Omega/\partial \mu \), expanding up to the second-order virial coefficient. We show also the zero-temperature result obtained from the local density approximation. The temperature dependence of the structure

\[
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\]
we expect that the scaled structure factor are now ready to determine the scaling region in which momenta and strong interactions, the scaled spin-antiparallel structure factor converges to the dimensionless contact $I/(Nk_F)$.

Inset in (a): a blow-up of the $T = 0$ scaled structure factor at the BEC-BCS crossover regime. In the universal region with large momenta and strong interactions, the scaled spin-antiparallel structure factor converges to the dimensionless contact $I/(Nk_F)$.

Universal scaling region of our Tan relation. – We are now ready to determine the scaling region in which we expect that the scaled structure factor $S_{T\uparrow\downarrow}(q)/\langle q \rangle$ becomes momentum independent and converges to the contact of the system. Figure 3 shows the scaled structure factors of a trapped Fermi gas at different transferred momenta and at low and high temperatures. On the BCS side, the scaled structure factor is rather insensitive to the varying momentum. We observe that the scaling limit can be easily reached at the BEC-BCS crossover regime ($|1/k_Fa| < 0.5$), at a relatively small momentum $q = 2k_F$. However, to access the scaling limit in a broader region of interaction strengths (i.e., $1/k_Fa < 2$), a larger momentum ($q = 5k_F$) is necessary.

Conclusion. – Based on the structure-factor Tan relation eq. (2), we present a systematic study of the static structure factor of an interacting Fermi gas near the BEC-BCS crossover at a transferred momentum $q > k_F$. The scaling region of the structure-factor Tan relation is clarified. These predictions can be readily checked in future Bragg experiments at crossover, either near the ground state or at finite temperatures.

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