Temperature and coupling dependence of the universal contact intensity
for an ultracold Fermi gas

F. Palestini, A. Perali, P. Pieri, and G. C. Strinati
Dipartimento di Fisica, Università di Camerino, I-62032 Camerino, Italy
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Physical properties of an ultracold Fermi gas in the temperature-coupling phase diagram can be characterized by the contact intensity \( C \), which enters the pair-correlation function at short distances and describes how the two-body problem merges into its surrounding. We show that the local order established by pairing fluctuations about the critical temperature \( T_c \) of the superfluid transition considerably enhances the contact \( C \) in a temperature range where pseudogap phenomena are maximal. Our \textit{ab initio} results for \( C \) in a trap compare well with recently available experimental data over a wide coupling range. An analysis is also provided for the effects of trap averaging on \( C \).

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The “contact” \( C \), introduced by Tan [1,2] to characterize the merging of two-body into many-body physics in systems like ultracold Fermi gases with a short-range interparticle interaction, has attracted much interest lately [3–7]. This is especially relevant in the context of the BCS-BEC crossover, whereby a smooth evolution occurs jointly for the two-body and many-body physics, from the presence of Cooper pairs with an underlying Fermi surface in the BCS limit, to the formation of molecular bosons with a residual interaction in the Bose-Einstein condensate (BEC) limit.

Recently, the contact \( C \) was measured in an ultracold gas of trapped fermionic \( ^{40}\text{K} \) atoms [8], from the large-momentum tail of the momentum distribution as well as from the high-frequency tail of the radio-frequency signal following an earlier suggestion [9]. These measurements were done from about unitarity (where the scattering length \( a_F \) of the Fano-Feshbach resonance diverges) to deep inside the BCS region (more precisely, in the coupling range \(-2.5 \leq (k_F a_F)^{-1} \leq +0.5 \)) where \( k_F = (2m E_F)^{1/2} \) is the Fermi wave vector expressed in terms of the Fermi energy \( E_F = \omega_0(3N^{1/2}) \), \( m \) being the atom mass, \( N \) the total number of atoms, and \( \omega_0 \) the average trap frequency [10], and in a temperature range about the critical temperature \( T_c \).

Several questions concerning the contact \( C \) remain open. They hinge on the recent experimental results of Ref. [8] (like the temperature and coupling dependence of \( C \), and the effect that trap averaging has on the values of \( C \)), as well as on more theoretical issues. These include the identification of the (approximate) spatial boundary between short-range and medium-range physics that can be associated with the contact \( C \), the effects that improved theoretical approaches have on the values of \( C \), and the interconnection with the presence of a pseudogap in the single-particle excitation spectrum.

In this paper, we address these questions and calculate the contact \( C \) using a \( t \)-matrix approach [11] that proved successful in comparison with data obtained from momentum-resolved radiofrequency spectroscopy to realize an analogue of photoemission spectroscopy for ultracold Fermi atoms [12], and also using a nontrivial extension of this theory [13] which takes into account the residual interaction among composite bosons. This is to verify to what an extent improvements on the description of the medium-range physics (over and above the results of the \( t \) matrix) influence the values of \( C \) in different coupling and temperature ranges [14].

We shall, specifically, be concerned with the temperature dependence of \( C \) over an extended temperature range up to (several times) the Fermi temperature \( T_F \) to determine how the value of \( C \) is affected by the pseudogap physics extending above \( T_c \) in the unitary \([-1 \leq (k_F a_F)^{-1} \leq +1\)] regime, and to address the related question of how trap averaging influences the value of \( C \) with respect to that of a homogeneous system with the same nominal temperature and coupling.

The contact \( C \) was originally introduced to account for the large wave-vector behavior of the fermionic distribution \( n(k) \) (for spin component) of the homogeneous system, such that \( n(k) \approx C \theta^k \). Here the suffix “\( h \)” stands for homogeneous, \( k = |k| \) is in units of \( k_F = (3\pi^2 n)^{1/3} \) where \( n \) is the total particle density, and \( n(k) \) is normalized such that \( \int\frac{d^3k}{(2\pi)^3} n(k) = 1/2 \). Alternatively, \( C_h \) can be extracted from the high-frequency tail of the radio-frequency (rf) spectrum \( I_{rf}(\omega) \) per unit volume, so that \( I_{rf}(\omega) \approx (C_h^2/2\pi^2 \hbar \omega)^{-3/2} \). Here the frequency \( \omega \) is in units of \( E_F \) and the rf spectrum is normalized such that \( \int_0^{\infty} d\omega I_{rf}(\omega) = 1/2 \). The above asymptotic form of \( I_{rf}(\omega) \) holds provided final-state effects can be neglected [9,15,16].

Similar asymptotic behaviors can be obtained for the trapped system. Preserving the above normalization as for the homogeneous system, we write within a local-density approximation

\[
n(k) = \int d\mathbf{r} n(k; \mathbf{r}) \approx \frac{C_i}{k^2},
\]

where

\[
C_i = \frac{8}{\pi^2} \int \frac{[3\pi^2 n(\mathbf{r})]^{4/3}}{k_F^4} C_h(\mathbf{r}).
\]

Here the suffix “\( t \)” and \( k_F \) refer to the trapped system, the spatial position \( \mathbf{r} \) is in units of the Thomas-Fermi radius \( R_F = [2E_F/(m_0 \omega_0^2)]^{1/2} \), and \( n(\mathbf{r}) \) and \( C_h(\mathbf{r}) \) are the density and contact locally in the trap. By a similar token, the large-\( \omega \) behavior of the total rf spectrum of the trapped system reduces to

\[
I_{rf}(\omega) = \int d\mathbf{r} I_{rf}(\omega; \mathbf{r}) \approx \frac{C_i}{2^{3/2} \pi^{1/2} \omega^{3/2}}.
\]

with the overall normalization of the homogeneous case.

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At unitarity vs coupling (light-dotted lines) as well as the dashed line. The leading approximations in weak and strong interaction among the composite bosons, is appreciable only close to unitarity where particles correlate with each other within the interparticle spacing \( k_F a_F \). The smallness of this difference resulting from our calculations confirms the validity of the \( t \)-matrix approximation for the contact \( C_h \) and for the high-energy scale to which \( C_h \) is associated. Yet this difference is relevant for the physical interpretation of the contact \( C_h \) as characterizing the effects of medium-range (many-body) physics over and above the short-range (two-body) physics. This interpretation is also consistent with rewriting \( C_h = (3\pi^2/4)(\Delta_{\infty}/E_F)^2 \) in terms of the high-energy scale \( \Delta_{\infty} \) introduced in Ref. [9], such that \( \Delta_{\infty} = 2\pi |a_F| n/m \) embodies in weak coupling the effects of surrounding particles through a mean-field shift [17], while \( \Delta_{\infty}^2 = 4\pi n/(m^2 a_F) \) reflects a standard relation in strong coupling [18] between the density and the gap parameter within BCS theory. For comparison, Fig. 1(a) also reports the coupling dependence of \( C_h \) at zero temperature (dashed-dotted line) within the \( t \)-matrix approximation, to which the above approximate expressions in the BCS and BEC limits converge. This dependence is in agreement with that obtained in Ref. [19] within a Gaussian pair-fluctuation theory.

Figure 1(b) shows the temperature dependence of \( C_h \) at unitarity over an extended temperature range within the \( t \)-matrix approximation. The rather slow decay of \( C_h \) at high temperature is consistent with the expectation that \( C_h \) is not related to long-range order. The temperature behavior of \( C_h \) steepens up at low temperature when entering the pseudogap region for \( T/T_F \lesssim 0.5 \) [12], thus evidencing the emergence of a local (medium-range) order which is also responsible for the pseudogap. Such an enhancement of the value of \( C_h \) appears most evident when the calculation is continued below \( T_c \) [20], with the result that a cusp appears in \( C_h \) at \( T_c \) where the effect of the pseudogap is maximum. To emphasize this enhancement, we have indicated in Fig. 1(b) the extrapolation of the high-temperature behavior of \( C_h \) (dashed line) down to \( T = 0 \), on top of which the contribution associated with the pseudogap region about \( T_c \) appears evident. Our value \((-3.23)\) for \( C_h \) at \( T = 0 \) compares well with that \((-3.40)\) extracted from the Monte-Carlo calculations ofRef. [21]. For completeness, the inset of Fig. 1(b) reports the temperature dependence of \( C_h \) for \( (k_F a_F)^{-1} = 1.0 \) (full line, left scale) and \( (k_F a_F)^{-1} = 1.0 \) (dashed line, right scale). The maximum at \( T/T_F \approx 0.5 \) in the weak-coupling curve is consistent with the Fermi-liquid behavior discussed in Ref. [14].

The temperature dependence of \( C_h \) is here reported for the first time and deserves further comments. On physical grounds, the enhancement of \( C_h \) when entering the fluctuative region above \( T_c \) is due to the strengthening of local pairing correlations in the absence of long-range order. In this respect, the most appealing definition of the contact is through the short-range behavior of the pair-correlation function between opposite spins [1]. This quantity is affected by pairing fluctuations in the particle-particle channel, of which the \( t \)-matrix represents the most important contribution. In addition, the contact \( C_h \), through its alternative definition in terms of the high-energy scale \( \Delta_{\infty} \) that was previously mentioned, can be related to a wave vector and frequency averaging of the pair-fluctuation propagator [9]. The wave-vector and frequency structures of the very same pair-fluctuation propagator also give rise to a characteristic low-energy scale \( \Delta_{pg} \) in the single-particle excitations [11], which is referred to as the pseudogap. The interdependence between the two energy scales \( \Delta_{\infty} \) and \( \Delta_{pg} \) can then be explicitly appreciated in Fig. 2, where they are shown at \( T_r \) versus the coupling

![Figure 1](image-url)

**FIG. 1.** (Color online) The contact \( C_h \) for the homogeneous case: (a) At \( T_c \) vs the coupling \((k_F a_F)^{-1}\), obtained within the \( t \)-matrix approximation (full line) and its improved Popov version (dashed line). The leading approximations in weak and strong coupling (light-dotted lines) as well as the \( T = 0 \) result within the \( t \)-matrix approximation (dashed-dotted line) are also reported. (b) At unitarity vs \( T/T_F \), obtained within the \( t \)-matrix (full line). The high-temperature approximation to this curve is also reported as a reference (dashed line) and extrapolated to \( T = 0 \). [See the text for the meaning of the inset.]
The inset shows, correspondingly, the characteristic value \( k_C \), note how numerical values recover the limiting ones obtained for a dilute Fermi gas [22].

In extreme weak coupling, our calculation at \( k_F a_F \)−1, the low-energy scale \( \Delta_\infty \) (normalized to \( \Delta k \)), at which the asymptotic power-law behavior \( n(k) \approx C_b k^{-4} \) is reached within 2.5% (dashed line), 5% (dashed-dotted line), and 10% (full line) accuracy, are shown at \( T_c \) versus \( (k_F a_F)^{-1} \). The inset shows, correspondingly, the characteristic value \( C_t \) (normalized to \( E_F \)), at which the asymptotic power-law behavior \( I_0(\omega) \approx (C_0/2^{3/2} \pi^2) \omega^{-3/2} \) of the rf spectrum is reached within 10% accuracy.

In addition, the inset of Fig. 3 shows the value of \( \omega_C \) at \( T_c \) versus \( (k_F a_F)^{-1} \), extracted within a 10% accuracy from the large-\( \omega \) behavior of the rf spectrum. (Recall that the \( \omega^{-3/2} \) tail of the rf spectrum originates from the short-range behavior of the two-body wave function [23,24] in the absence of final-state effects [25].) A comparison with \( k_C \) with the same accuracy yields the relation \( 2\omega_C = k_C^2 \) that holds approximately for all couplings.

The values of the contact \( C_t \) obtained from Eq. (1), by adding the asymptotic contributions from all shells in the trap within the \( t \)-matrix approximation, are reported in Fig. 4 at \( T_c \) versus \( (k_F a_F)^{-1} \) (full line). They are compared with the values (filled and empty circles, stars) obtained experimentally in Ref. [8] through alternative procedures. Note that in the experiment the system is above (below) \( T_c \) in the BCS (BEC) side of the unitary region. The theoretical value obtained at unitarity for \( T = 0 \) is also reported for comparison (empty square). Due to difficulties in extracting the asymptotic behavior of \( n(k) \) from experimental data, the figure also shows the theoretical values of \( C_t \) (dashed-dotted line) obtained upon averaging \( k^4 n(k) \) over the interval \( k_{min} \leq k \leq k_{max} \). This follows the procedure used to extract the experimental values of \( C_t \), for which \( k_{min} = 1.55 \) when \( (k_F a_F)^{-1} < -0.5 \) and \( k_{min} = 1.85 \) when \( -0.5 < (k_F a_F)^{-1} \), while \( k_{max} = 2.5 \) [8].

It is worth noting that the data of Ref. [8] which are reported in Fig. 4, have been originally compared with a theoretical curve from Ref. [4], where the behavior of \( C_t \) at \( T = 0 \) was obtained across the unitary regime by interpolating known results in the BCS and BEC limits. That interpolation has to be contrasted with the completely \textit{ab initio} theoretical calculation at \( T = 0 \) reported by the full line in Fig. 4, which spans a wide coupling range just across the unitary regime. A similar calculation at \( T = 0 \) within a Gaussian pair-fluctuation theory has been reported in Ref. [19].

Finally, the inset of Fig. 4 displays the temperature dependence of \( C_t \) for the trapped case at unitarity within the \( t \)-matrix approximation (full line), with the vertical arrow indicating the corresponding value of \( T_c \). Contrary to the result for the homogeneous case of Fig. 1(b), no cusp now appears in \( C_t \) at \( T_c \) for the trapped case. An expanded discussion about the effects that trap averaging has on the values of \( C_t \) is provided.
In addition, we note that for \( T > T_F \) we retrieve the \( T^{-5/2} \) dependence reported in Ref. [27], while for \( T < T_F \) our results somewhat differ from the (high-temperature) virial expansion of Ref. [19].

In conclusion, we have presented a detailed analysis of the contact intensity \( C \) for a Fermi gas over the temperature-coupling phase diagram. The values of \( C \) have been obtained from the large-\( k \) behavior of the momentum distribution \( n(k) \) as well as from the large-\( \omega \) tail of the rf spectrum \( I_{rf}(\omega) \), both for the homogeneous and trapped case. For the latter case, good agreement is obtained with recent experimental data. The effects of pairing fluctuations on \( C \) have been determined by the \( t \)-matrix approximation and its improved Popov version that takes into account the interaction among composite bosons. We have found that the values of \( C \) are strongly affected by the emergence of a pseudogap in the single-particle excitations about \( T_c \).

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