Exact Relations for a Strongly-interacting Fermi Gas from the Operator Product Expansion

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The momentum distribution in a Fermi gas with two spin states and a large scattering length has a tail that falls off like $1/k^4$ at large momentum $k$, as pointed out by Shina Tan. He used novel methods to derive exact relations between the coefficient of the tail in the momentum distribution and various other properties of the system. We present simple derivations of these relations using the operator product expansion for quantum fields. We identify the coefficient as the integral over space of the expectation value of a local operator that measures the density of pairs.

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Many-body systems of fermions have long been of great importance in astrophysics, nuclear physics, and solid state physics. The development of trapping and cooling techniques for ultracold atoms has made them important in atomic physics as well. In this case, the strength of the interaction is governed by the 2-body scattering length which can be controlled experimentally, adding a new dimension to the problem.\[1]\]

If the scattering length $a$ is much larger than the range of the interactions, the system has universal properties that are determined only by the large scattering length. For sufficiently low number density $n$, the universal properties can be calculated using perturbative methods. If $n[a]^3$ is comparable to 1 or larger, the problem becomes nonperturbative. In the special case of two equally-populated spin states, systematically improvable calculations are possible using Monte Carlo methods. If the populations are not equal, this approach suffers from the fermion sign problem. If there are 3 or more spin states, the problem is complicated by the Efimov effect.\[2]\] The challenging nature of the general problem makes exact results very valuable. One case in which exact results are known is the unitary limit $a = \pm\infty$, where they can be derived by exploiting scale invariance and conformal invariance.\[3]\]

In 2005, Shina Tan pointed out that the momentum distribution in an arbitrary system consisting of fermions in two spin states with a large scattering length has a large-momentum tail that falls off as $1/k^4$,\[4]\] The number of fermions with momentum larger than $K$ approaches $C/(\pi^2 K)$ as $K \rightarrow \infty$, where $C$ depends on the state of the system. Tan used novel methods involving generalized functions to derive exact relations between $C$ and several other properties of the system. An example is the adiabatic relation that gives the change in the total energy $E$ due to a small change in $a$:\[5]\]

$$\frac{dE}{d(1/a)} = -\frac{\hbar^2}{4\pi m} C. \quad (1)$$

Tan referred to $C$ as the integrated contact intensity, which we will abbreviate to contact. The Tan relations hold for any state of the system: few-body or many-body, homogeneous or in a trapping potential, superfluid or normal, zero or nonzero temperature.

In this Letter, we show that the Tan relations can be derived using the operator product expansion (OPE) for quantum fields. The OPE was proposed by Ken Wilson in 1969 as a formalism for dealing with the strong interactions associated with the nuclear force. The OPE has become a standard tool to understand the relativistic quantum field theories that describe elementary particles.\[6]\] We will apply the OPE to the strongly-interacting nonrelativistic system consisting of fermions with two spin states and a large scattering length. We identify the contact $C$ as the expectation value of the integral over space of a local operator that measures the density of pairs. The OPE provides new insights into the Tan relations and makes it easier to generalize them to systems with additional degrees of freedom or more complicated interactions.

A system consisting of fermions in two spin states labeled by $\sigma = 1, 2$ can be described by a quantum field theory with two quantum fields $\psi_\sigma(r)$. The number operator is $\sum_\sigma \int d^3 R \psi_\sigma^\dagger(R) \psi_\sigma(R)$. The momentum distribution $\rho_\sigma(k)$ for fermions with spin $\sigma$ can be expressed as

$$\rho_\sigma(k) = \int d^3 R \int d^3 r \, e^{ik \cdot r} \langle \psi_\sigma(R + \frac{1}{2}r) \psi_\sigma(R - \frac{1}{2}r) \rangle. \quad (2)$$

Its behavior at large $k$ is determined by the matrix element at small $r$. If the fermions are non-interacting, the quantum fields can be expanded as Taylor series in $r$. The resulting expansion for $\rho_\sigma(k)$ can be expressed in terms of the Dirac delta function in $k$ and derivatives of the delta function. This indicates that $\rho_\sigma(k)$ has a finite range in $k$. Simple examples are an ideal gas of fermions at 0 temperature, for which $\rho_\sigma(k)$ vanishes if $|k|$ is larger than the Fermi momentum, and an ideal gas of fermions
at high temperature, for which $\rho_\sigma(k)$ is a Gaussian function of $k$.

If there are interactions between the fermions, the matrix element in Eq. (2) may not be an analytic function of $r = 0$. The momentum distribution $\rho_\sigma(k)$ may therefore have a large-momentum tail that falls off like a power of $k = |k|$. Tan showed that for fermions with two spin states and a large scattering length, the tail is proportional to $1/k^4$ and is the same for both spin states:

$$\rho_\sigma(k) \rightarrow C/k^4, \quad (3)$$

where $C$ is the contact. This power-law behavior can arise from a term in the matrix element in Eq. (2) that is linear in $r = |r|$ as $r \rightarrow 0$. It holds for all states that include at least one particle of each spin. The dependence on the state enters only through $C$.

The possibility of a power-law tail in the momentum distribution can be understood from Wilson’s OPE. Wilson proposed that in a quantum field theory a product of local operators separated by a short distance can be expanded in terms of local operators.

The functions $C_{\sigma,n}(r)$ are called Wilson coefficients or short-distance coefficients. Some of them can be non-analytic at $r = 0$, so the momentum distribution $\rho_\sigma(k)$ can have a power-law tail.

The Hamiltonian density for the quantum field theory that describes fermions with two spin states and a large scattering length in an external potential $V(R)$ is

$$\mathcal{H} = \sum_\sigma \frac{1}{2m} \nabla \psi_\sigma^\dagger \cdot \nabla \psi_\sigma + \frac{g(\Lambda)}{m} \psi_1^\dagger \psi_2^\dagger \psi_1 \psi_2 + V, \quad (5)$$

where $V = V(R) \sum_\sigma \psi_\sigma^\dagger \psi_\sigma$. For simplicity, we have set $\hbar = 1$. The superscripts $(\Lambda)$ on the operators in Eq. (5) indicate that their matrix elements are ultraviolet divergent and an ultraviolet cutoff is required to make them well defined. For the ultraviolet cutoff, we impose an upper limit $|k| < \Lambda$ on momentum integrals. In the limit $\Lambda \rightarrow \infty$, the Hamiltonian density in Eq. (5) describes fermions with zero-range interactions and scattering length $a$ if we take the coupling constant to be

$$g(\Lambda) = \frac{4\pi a}{1 - 2a\Lambda/\pi}. \quad (6)$$

The amplitude for the scattering of a pair of fermions can be calculated by solving the Lippmann-Schwinger integral equation, which is represented diagrammatically in Fig. 1. The solution $A(E)$ depends on the total energy $E$ of the pair of fermions in the center-of-mass frame and not separately on their momenta. After substituting $\Theta_k$ for $\Lambda$, the solution in the limit $\Lambda \rightarrow \infty$ is

$$A(E) = \frac{4\pi/m}{1/a + \sqrt{mE - \epsilon}}. \quad (7)$$

The T-matrix element for scattering of a pair of fermions with momenta $+p$ and $-p$ is obtained by setting $E = p^2/m$.

We now proceed to show that the OPE in Eq. (1) includes a term with the operator $O_{12} = \psi_1^\dagger \psi_2^\dagger \psi_1 \psi_2$ and that its Wilson coefficient $C_{12}(r)$ is linear in $r = |r|$. Since the OPE is an operator equation, $C_{12}(r)$ can be determined by calculating the expectation value of both sides of the OPE in the simplest states for which $\langle \psi_1^\dagger \psi_2^\dagger \psi_1 \psi_2 \rangle$ is nonzero. We choose the state $|\pm p\rangle$ consisting of two fermions with spins 1 and 2 and with momenta $+p$ and $-p$.

We first consider the left side of the OPE in Eq. (1). The operator product at $R = 0$ can be represented diagrammatically by a pair of dots that correspond to the points $+\frac{1}{2}r$ and $-\frac{1}{2}r$ where it annihilates an incoming fermion and creates an outgoing fermion. The expectation value can be represented by the sum of the diagrams in Fig. 1(a) and the three diagrams with one or no scatterings. The contributions from the other three diagrams
are analytic at \( r = 0 \). The contribution from the diagram in Fig. 2(a) is
\[
\langle \psi_k^\dagger (-\frac{1}{r}) \psi_\sigma (\frac{1}{r}) \rangle_{\pm p} \bigg|_{\text{Graph}2(a)} = im^2 A^2 (p^2/m) e^{ipr}/(8\pi p) .
\]
(8)

If we expand this in powers of \( r \), the terms with odd powers of \( r \) are nonanalytic at \( r = 0 \).

We now consider the right side of the OPE in Eq. (4). The expectation value of \( \psi_k^\dagger \psi_\sigma \) can be represented by the sum of the diagram in Fig. 2(b) and the three diagrams with one or no scatterings. The contribution from the diagram in Fig. 2(b) is
\[
\langle \psi_k^\dagger \psi_\sigma (0) \rangle_{\pm p} \bigg|_{\text{Graph}2(b)} = im^2 A^2 (p^2/m)/(8\pi p) .
\]
(9)
This matches the \( r^0 \) term in the expansion of Eq. (8) in powers of \( r \). Thus we find that the Wilson coefficient of \( \psi_k^\dagger \psi_\sigma (R) \) in Eq. (4) is simply \( 1 \) in accord with naive expectations. To match the term linear in \( r \) in the expansion of Eq. (8), we must find an operator whose expectation value in the state \( \pm p \) has the momentum dependence \( A^2 (p^2/m) \). One can deduce this operator by realizing that the nonanalytic behavior at \( r = 0 \) must arise from the region of the diagram in Fig. 2(a) in which there is large momentum flowing in the lines that connect the operators to the amplitudes and the line that connects the two amplitudes. If we shrink all these lines to a point, they reduce to a vertex with two incoming lines and two outgoing lines. The simplest corresponding operator is \( \mathcal{O}_{12} = \psi_1^\dagger \psi_2^\dagger \psi_1 \psi_2^\dagger (A) \). We can verify that this is the correct operator by calculating its matrix element, which can be represented by the sum of the diagram in Fig. 2(c) and the three diagrams with one or no scatterings. By using the integral equation in Fig. 1 the sum of the four diagrams can be expressed in the simple form
\[
\langle \psi_1^\dagger \psi_2^\dagger \psi_1 \psi_2^\dagger (A) (0) \rangle_{\pm p} = m^2 g^2 (\Lambda) A^2 (p^2/m) .
\]
(10)
This has the same dependence on \( p \) as the term linear in \( r \) in the expansion of Eq. (8). To match this term, the Wilson coefficient must be \( C_{\sigma, 12}(r) = -g^2 (\Lambda) / (8\pi) \). The expectation value of the term in OPE can be written
\[
C_{\sigma, 12}(r) \langle \mathcal{O}_{12} (R) \rangle = \frac{r}{8\pi} (g^2 \psi_1^\dagger \psi_1 \psi_2^\dagger \psi_2 (R) ) .
\]
(11)
We have attached the factor \( g^2 (\Lambda) \) to the operator \( \psi_1^\dagger \psi_2^\dagger \psi_1 \psi_2^\dagger (A) \) and suppressed the dependence on \( \Lambda \), because the resulting operator has finite matrix elements in the limit \( \Lambda \to \infty \), as exemplified by Eq. (11). We proceed to use this result to derive the Tan relations.

**Tail of the momentum distribution.** The leading behavior of \( \rho_{\sigma} (k) \) at large \( k \) can be obtained by inserting the term in Eq. (11) in place of the matrix element in Eq. (8). This term gives the asymptotic behavior in Eq. (8) with
\[
C = \int d^3 R \left( g^2 \psi_1^\dagger \psi_1 \psi_2^\dagger \psi_2 (R) \right) .
\]
(12)
We will refer to \( g^2 \psi_1^\dagger \psi_1 \psi_2^\dagger \psi_2 \) as the contact density operator. This is a positive operator, so \( C \geq 0 \).

**Energy relation.** In Ref. [8], Shina Tan derived an expression for the energy \( E \) as a linear functional of the momentum distributions:
\[
E = \sum_{\sigma} \int \frac{d^3 k}{(2\pi)^3} \frac{k^2}{2m} \left( \rho_{\sigma} (k) - \frac{C}{k^4} \right) + \frac{C}{4\pi ma} + \int d^3 R \langle V \rangle .
\]
(13)
This is a functional of \( \rho_1 \) and \( \rho_2 \), because \( C \) is determined by their large-momentum behavior: \( C = \lim_{k \to \infty} k^4 \rho_{\sigma} (k) \). Tan’s energy relation can be derived simply by using the expression for \( g (\Lambda) \) in Eq. (10) to express the Hamiltonian density in Eq. (11) as the sum of three terms whose matrix elements are ultraviolet finite:
\[
\mathcal{H} = \left( \sum_{\sigma} \frac{1}{2m} \nabla \psi_1^\dagger \cdot \nabla \psi_2 (A) - \frac{m A}{2\pi^2} g^2 \psi_1^\dagger \psi_1 \psi_2 + V \right) .
\]
(14)
The operator \( \nabla \psi_1^\dagger \cdot \nabla \psi_2 (A) \) in the first term has matrix elements that diverge linearly as \( \Lambda \to \infty \). This linear divergence is cancelled by the second term, which has an explicit factor of \( \Lambda \). Integrating over the positions of the local operators in Eq. (14), taking the expectation value, and using the expression for \( C \) in Eq. (12), we obtain Tan’s energy relation in Eq. (13).

**Adiabatic relation.** Eq. (11) can be derived by using the Feynman-Hellman theorem:
\[
dE/da = \int d^3 R \langle \partial \mathcal{H} / \partial a \rangle .
\]
(15)
Since \( \mathcal{H} \) depends on \( a \) only through the coupling constant \( g (\Lambda) \) in Eq. (9), its derivative can be written
\[
\partial \mathcal{H} / \partial a = g^2 \psi_1^\dagger \psi_1 \psi_2^\dagger \psi_2/(4\pi ma^2) .
\]
(16)
Upon inserting this into Eq. (15) and using Eq. (12) for \( C \), we get the adiabatic relation in Eq. (1).

**Virial theorem.** The virial theorem for fermions with two spin states in a harmonic trapping potential in the unitary limit \( a = \pm \infty \) was derived in Ref. [10]. Tan has derived a generalization of the virial theorem for the case of finite \( a \) [11]. The virial theorem can be derived more simply by using the fact that the scattering length \( a \) and the angular frequency \( \omega \) of the trapping potential provide the only scales for the energy \( E \) of a state. Dimensional analysis then requires the differential operator \( (\omega \partial / \partial \omega) - \frac{1}{2} (a \partial / \partial a) \) to give 1 when acting on \( \int d^3 R \langle \mathcal{H} \rangle \). Using the Feynman-Hellman theorem together with Eq. (16), we obtain the virial theorem
\[
E = 2 \int d^3 R \langle V \rangle - C / (8\pi ma) .
\]
(17)
We can obtain a simple interpretation of the contact density operator by considering the OPE of the number
density operators $\psi_1^\dagger \psi_2(\pm \mathbf{r})$ and $\psi_1^\dagger \psi_2(+\mathbf{r})$. The expectation value of their product in the state $|\pm \mathbf{p}\rangle$ can be represented by the sum of the diagram in Fig. 2(d) and the three diagrams with one or no scatterings. The contribution that is most singular as $r \to 0$ comes from the diagram in Fig. 2(d): $m^2 A^2(\gamma^2/m)e^{2i\pi r}/(16\pi^2 r^3)$. The term proportional to $r^{-2}$ has the same dependence on $p$ as the matrix element in Eq. (10). Thus the most singular term in the OPE is

$$\psi_1^\dagger \psi_2(\mathbf{R} - \mathbf{r})\psi_1^\dagger \psi_2(\mathbf{R} + \mathbf{r}) \to \frac{1}{16\pi^2} g^2 \psi_1^\dagger \psi_1^\dagger \psi_2^\dagger \psi_2(\mathbf{R}).$$

(18)

We can define an operator $N_{\text{pair}}(\mathbf{R}, s)$ that counts the number of pairs of fermions with spins 1 and 2 near the point $\mathbf{R}$ with separation less than $s$ by integrating the left side of Eq. (18) over the ball $|\mathbf{r}| < s$. In the absence of interactions, $\langle N_{\text{pair}}(\mathbf{R}, s) \rangle$ scales as $s^2$ as $s \to 0$. Eq. (18) implies that in the case of a large scattering length $\langle N_{\text{pair}}(\mathbf{R}, s) \rangle$ scales as $s^4$. We can interpret the contact density operator $g^2 \psi_1^\dagger \psi_2^\dagger \psi_1 \psi_2$ as the limit as $s \to 0$ of $(4\pi/s) N_{\text{pair}}(\mathbf{R}, s)$.

One can give a more intuitive interpretation of the contact $C$ if the fermions with spins 1 and 2 have an inelastic two-body scattering channel into other spin states that are much lower in energy. In this case, the optical theorem implies that the scattering length $a$ has a negative imaginary part. The leading effects of a weakly-coupled inelastic channel on low-energy fermions in the spin states of interest can be taken into account through the small imaginary part of $a$. The effect on a state with definite energy $E$ is to change its time-dependence from $\exp(-iEt/h)$ to $\exp(-(iE - i\Gamma/2)t/h)$. The probability in that state decreases with time at the rate $\Gamma/h$. The adiabatic relation in Eq. (11) can be used to derive an expression for $\Gamma$ to leading order in the imaginary part of $a$:

$$\Gamma \approx \frac{\hbar^2 (-\text{Im } a)}{2\pi m|a|^2} C.$$

(19)

Thus $C$ determines the rate at which low-energy fermions are depleted by inelastic collisions.

In Ref. [6], Tan derived expressions for the contact density in the BCS limit ($a \to 0^-$), the unitary limit ($a \to \pm \infty$), and the BEC limit ($a \to 0^+$) by using the adiabatic relation in Eq. (11) as an operational definition of $C$. Our identification of the local contact density operator $g^2 \psi_1^\dagger \psi_2^\dagger \psi_1 \psi_2$ makes it straightforward to calculate the contact density for homogeneous systems directly using diagrammatic methods.

The Tan relations for ultracold fermionic atoms with two spin states apply equally well to cold neutron matter at sufficiently low densities. One advantage of our derivation using the OPE is that it makes it easier to generalize the Tan relations to more complicated systems. The generalization to more complicated interactions is straightforward for any system that can be described by a renormalizable local quantum field theory [12]. An important example is the resonance model that provides a natural description of atoms near a Feshbach resonance [13]. The generalization to systems with additional spin degrees of freedom, such as nuclear matter at sufficiently low densities, is complicated by the Efimov effect [2]. In such cases, a 3-body analog of the contact density operator may be expected to play an important role.

The original definition of the contact $C$ in terms of the tail of the momentum distribution suggests that the Tan relations are relevant only to esoteric aspects of the strongly-interacting Fermi gas. However the adiabatic relation in Eq. (11) and the virial theorem in Eq. (17) make it clear that they are actually of central importance. In Refs. [3, 6], Tan offered suggestions for how these relations could be tested experimentally. We leave this as a challenge to the ingenuity of experimentalists in cold atom physics.

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