Momentum Distribution and Contact of the Unitary Fermi gas

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We calculate the momentum distribution $n(k)$ of the Unitary Fermi Gas using Quantum Monte Carlo calculations at finite temperature $T/\varepsilon_F$ as well as in the ground state. At large momenta $k/k_F$, we find that $n(k)$ falls off as $C/k^3$, in agreement with the Tan relations. From the asymptotics of $n(k)$, we determine the contact $C$ as a function of $T/\varepsilon_F$ and present a comparison with theory. At low $T/\varepsilon_F$, we find that $C$ increases with temperature, and we tentatively identify a maximum around $T/\varepsilon_F \simeq 0.4$. Our calculations are performed on lattices of spatial extent up to $N_x = 14$ with a particle number per unit volume of $\simeq 0.03 - 0.07$.

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The Unitary Fermi Gas (UFG) is one of the most interesting strongly interacting systems known to date, as it saturates the unitarity bound on the quantum mechanical scattering cross section $\sigma_0 \leq 4\pi/k^2$. Since the proposal of the UFG as a model for dilute neutron matter by Bertsch \cite{bertsch} and its realization in ultracold atom experiments \cite{anderson}, the UFG has garnered widespread attention across multiple disciplines, including atomic physics \cite{bloch}, nuclear structure \cite{layne} and relativistic heavy-ion collisions \cite{wilson}. The UFG is defined as a two-component many-fermion system in the limit of short interaction range $r_0$ and large $s$-wave scattering length $a$,

$$0 \leftarrow k_F r_0 \ll 1 \ll k_F a \rightarrow \infty,$$

with $k_F \equiv (3\pi^2 n)^{1/3}$ the Fermi momentum and $n$ the particle number density. The special properties of the UFG arise from the fact that it is characterized by a single scale, given by the inter-particle distance $\sim k_F^{-1}$, without reference to the details of the interaction. While the thermodynamic properties of the UFG are universal \cite{drut}, the lack of an obvious dimensionless expansion parameter makes the UFG a challenging many-body problem.

In spite of the challenges of the unitary limit, much progress has been made with purely analytical methods. Notably, in 2005 Tan was able to derive exact thermodynamic relations \cite{tan} in terms of a universal quantity known as the “contact” $C$, which determines the number of pairs separated by short distances. Since then, the Tan relations have been re-derived in multiple ways \cite{tan,harada,levelt} as well as in the ground state. At large momenta $k/k_F$, the Tan relations (as well as the above-mentioned sum rules) remain valid at arbitrary $k_F a$ as long as $k_F r_0 \ll 1$. For further details and a comprehensive review, see Ref. \cite{drut}.

The calculation of $C$ itself, however, remains a challenge, as it depends on the intricate many-body dynamics of the unitary regime. In principle, $C$ can be extracted from any one of the Tan relations (as recently done in experiments \cite{tan}). One of the simplest relations concerns the asymptotics of the momentum distribution, and asserts that

$$C \equiv \lim_{k \rightarrow \infty} k^4 n_\sigma(k), \quad n_\sigma(k) = \langle \hat{a}_{\sigma,k}^\dagger \hat{a}_{\sigma,k} \rangle,$$

where $n_\sigma(k)$ is the momentum distribution expressed as a thermal average, and the $\hat{a}_{\sigma,k}$ and $\hat{a}_{\sigma,k}^\dagger$ denote creation and annihilation operators for particles of momentum $k$ and spin $\sigma$. If $n_\sigma(k)$ is normalized to the particle number $N_\sigma$, then $C$ is an extensive quantity with dimensions of momentum. We shall consider $C$ in units of $k_F$ divided by the total particle number $N = N_\uparrow + N_\downarrow$.

In this work, we focus on the momentum distribution of the homogeneous UFG and the extraction of $C$ via Eq. (2), using a Quantum Monte Carlo (QMC) approach which accounts fully for quantum and thermal fluctuations. On a spatial lattice, the Hamiltonian that captures the physics of the unitary limit can be written as

$$\hat{H} \equiv \sum_k \frac{\hbar^2 k^2}{2m} (\hat{a}_{\uparrow,k}^\dagger \hat{a}_{\uparrow,k} + \hat{a}_{\downarrow,k}^\dagger \hat{a}_{\downarrow,k}) - g \sum \hat{n}_{\uparrow,i} \hat{n}_{\downarrow,i},$$

where $m$ is the mass of the fermions (henceforth set to unity), $g$ is the bare coupling, and $\hat{n}_{\sigma,i}$ denotes the number density operator for spin projection $\sigma$ at lattice position $i$. The equilibrium thermodynamical properties are
obtained from the grand canonical partition function
\[ Z \equiv \text{Tr } \exp[-\beta(\hat{H} - \mu \hat{N})], \tag{4} \]
where \( \beta \equiv 1/k_BT \), \( \mu \) is the chemical potential, and
\[ \hat{N} \equiv \hat{N}_\uparrow + \hat{N}_\downarrow = \sum_i \hat{n}_{i\uparrow} + \sum_i \hat{n}_{i\downarrow}, \tag{5} \]
denotes the particle number operator.

In our QMC treatment, the system is placed on a \((3 + 1)\)-dimensional Euclidean space-time lattice via a Suzuki-Trotter decomposition of the Boltzmann weight in Eq. (4), and the interaction is represented via a Hubbard-Stratonovich (HS) transformation \[17\]. As we focus on the spin-symmetric case, the fermion sign problem is absent. The resulting path integral formulation is an exact representation of the many-body problem of Eq. (2), up to finite volume and discretization effects. These may be addressed by varying the spatial lattice volume \( V = N_x^3 \) and the density \( n \), such that the thermodynamic and continuum limits are recovered as \( V \to \infty \) and \( n \to 0 \). The latter requires great care, as too low densities imply a departure from the thermodynamic limit. We find that \( n \approx 0.03 - 0.05 \) particles per unit volume yield results accurate to \( \approx 7\% \) at finite temperature, and to \( \leq 5\% \) at \( T = 0 \).

Our lattice formulation is very similar to Ref. \[18\], but differs in at least three notable aspects. Firstly, we determine the bare lattice coupling constant \( g \) corresponding to the unitary regime by using Lüscher’s formula \[19\] as in Ref. \[21\]. This procedure yields \( g \approx 5.14 \) in the unitary limit. Secondly, we use the compact, continuous HS transformation
\[ \exp (\tau g \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\sigma_i \left[ 1 + B \sin(\sigma_i) \hat{n}_{i\uparrow} \right] \times \left[ 1 + B \sin(\sigma_i) \hat{n}_{i\downarrow} \right], \tag{6} \]
where \( \sigma_i \) (not to be confused with the spin projection) is the HS auxiliary field, with \( B^2/2 = \exp(\tau g) - 1 \), and \( \tau \) denotes the lattice spacing in the imaginary time direction. We find that \( \tau \approx 0.05 \) is sufficiently small to render discretization errors from the Suzuki-Trotter decomposition insignificant (see also Fig. 2). The above representation (referred to as “Type 4” in Ref. \[21\]) was found to be superior with respect to acceptance rate, decorrelation and signal-to-noise properties than the more conventional unbounded and discrete forms \[22\]. Thirdly, we update the auxiliary field \( \sigma \) by using the Hybrid Monte Carlo (HMC) algorithm \[23\] (familiar from Lattice QCD), which combines the Metropolis algorithm with deterministic Molecular Dynamics. Our implementation of the HMC algorithm enables global updates at all temperatures and lattice sizes, and scales approximately as \( \sim V^2 \) as a function of the spatial lattice volume, to be contrasted with the \( \sim V^3 \) scaling of approaches based on local updates.

We have performed calculations at \( T = 0 \) as well as \( T/\epsilon_F > 0 \), in the former case using an approach similar to Ref. \[21\]. Our main results correspond to \( 40 - 50 \) particles at \( N_x = 10 \) and \( 70 - 80 \) particles at \( N_x = 12 \), in addition to limited data for \( N_x = 14 \). In Fig. 1 we show the momentum distribution \( n(k) \) as a function of \( T/\epsilon_F \). We have computed \( n(k) \) by averaging over the angular directions on the lattice as well as over the imaginary-time slices. In this way, we find that \( \sim 200 \) uncorrelated auxiliary field samples for each datapoint gives excellent statistics for \( n(k) \). Multiplying \( n(k) \) by \( k^4 \), as plotted in Fig. 2, we find a peak at \( k \approx k_F \) and a leveling out at high momenta, with the asymptotic regime setting in at \( k \approx 2k_F \) at the lowest temperatures. It is fortuitous that the asymptotic regime sets in at such low momenta, as there is no obvious reason for this to be the case. It is then possible to study the temperature dependence of this “plateau”, which allows for a determination of the contact \( C/(Nk_F^4) \) as a function of \( T/\epsilon_F \). These results are given in Fig. 3 together with a comparison with available theoretical analyses. Our results indicate that \( n(k) \) follows the expected \( \sim k^{-4} \) dependence very accurately up to at least \( k \approx 4k_F \), at which point the signal deteriorates due to lattice artifacts.

The value of \( C \) in the ground state can be computed via Diffusion Monte Carlo (DMC) calculations, as first done in Ref. \[21\] using density-density correlations, which yielded \( C(T = 0)/(Nk_F^4) \approx 3.4 \), up to errors associated with fixing the nodes of the wavefunction. A more-
cent and comprehensive DMC calculation [25] came to the same conclusion using the equation of state, the momentum distribution and the density-density correlation. In contrast, our present results indicate that \( C(T = 0)/(Nk_F) \approx 2.95 \pm 0.10 \). The cause of this disagreement is being explored. The main sources of uncertainty in our determination of \( C/(Nk_F) \) are due to finite density effects. While we find that such effects tend to overestimate \( C/(Nk_F) \) as well as degrade the formation of an asymptotic \( \sim k^{-4} \) tail in \( n(k) \) at larger values of \( T/\epsilon_F \), larger lattices are needed in order to maintain the thermodynamic limit at lower densities.

The temperature dependence of \( C \) at unitarity was first determined analytically in Ref. [26], who considered two different limits. At very low temperatures \( T \ll T_c \approx 0.15\epsilon_F \), the dominant excitations are of phononic origin, and the \( T \)-dependence of \( C \) is of the form \( C/(Nk_F) \propto (T/\epsilon_F)^4 \). On the other hand, at very high temperatures \( T \gg \epsilon_F \), one finds \( C/(Nk_F) \approx 16/3 (\epsilon_F/T) \) within the second-order virial expansion. An interpolation between these limits then suggests that \( C(T/\epsilon_F) \) should present a maximum for \( T \sim \epsilon_F \). Recently, \( C \) has also been computed using two different types of \( t \)-matrix approximations [27, 28], as well as a third-order virial expansion [24]. The latter has shown evidence for convergence of the virial expansion down to \( T \sim \epsilon_F \). In light of these findings and upon analysis of various model calculations at low \( T \), Ref. [24] conjectured that the contact is likely a monotonically decreasing function of \( T \), except possibly in the phononic regime at very low \( T \). While the virial expansion is on solid ground at high \( T \), where it agrees with the \( t \)-matrix approaches of Refs. [27, 28], the actual \( T \)-dependence in the strongly correlated low-\( T \) regime has remained an open question, particularly since the UFG is strongly correlated even above \( T_c \) [30].

Our results show that \( C \) grows with \( T \) well beyond the superfluid phase, and are suggestive of a maximum \( C_{\text{max}} \approx 3.4 \) at \( T/\epsilon_F \approx 0.4 \). This scenario is in qualitative agreement with Ref. [24], as well as the \( t \)-matrix calculation of Ref. [27]. As \( C \) measures the number of particle pairs (of both spins) whose separation is small, the appearance of a maximum indicates an enhancement in such short-range correlations. This may be a result of local pairing order [27], which in turn suggests that \( C_{\text{max}} \) is directly related to pairing above \( T_c \), i.e. to a pseudogap. We find the scale at which the \( k^{-4} \) law sets in [see Fig. 2] to be \( k \approx 2k_F \) at finite \( T/\epsilon_F \) and somewhat lower for the ground state, in agreement with Ref. [12].

This universal property of the unitary limit characterizes the “healing distance” of the two-particle boundary condition on the many-body wavefunction, and therefore separates the microscopic properties from the universal macroscopic aspects of the unitary regime. Direct comparison of our data with ultracold atom experiments can be achieved by means of the virial expansion and the Local Density Approximation (LDA). While we defer this issue to a follow-up paper, we note that in light of the work of Ref. [31], the features of \( C(T/\epsilon_F) \) found in this study are unlikely to conflict with current experiments.
In summary, we have computed the momentum distribution $n(k)$ and the contact $C/(Nk_F)$ for the UFG at zero and finite $T/\epsilon_F$, using the auxiliary field QMC method in conjunction with the HMC algorithm. While the ground-state momentum distribution was first determined via DMC calculations in Ref. 32, our results represent the first fully non-perturbative calculation of $n(k)$ free of uncontrolled approximations. We find that the contact at $T = 0$ assumes the value $\approx 2.95 \pm 0.10$ and increases as a function of $T/\epsilon_F$ in the low- and intermediate temperature regimes that we have explored, which is consistent with the phononic scenario. Notably, DMC calculations find a somewhat larger value of $C/(Nk_F) \approx 3.4$, while the analytic approach of Ref. 26, which interpolates smoothly between the strong- and weak-coupling limits, yields $C/(Nk_F) \approx 3.0$ which is consistent with our data. Our results complement the calculations of Refs. 26–29 and are suggestive of a maximum consistent with our data. Our results complement the calculations at higher $C/(Nk_F)$ determined via DMC calculations in Ref. [32], our results

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