Momentum Distribution and Contact of the Unitary Fermi Gas

Joaquín E. Drut,[1,2] Timo A. Lähde,[3] and Timour Ten[1,4]
[1]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545-0001, USA
[2]Department of Physics, The Ohio State University, Columbus, Ohio 43210-1117, USA
[3]Helsinki Institute of Physics and Department of Applied Physics, Aalto University, FI-00076 Aalto, Espoo, Finland
[4]Department of Physics, University of Illinois, Chicago, Illinois 60607-7059, USA
(Received 8 January 2011; revised manuscript received 11 April 2011; published 20 May 2011)

We calculate the momentum distribution $n(k)$ of the unitary Fermi gas by using quantum Monte Carlo calculations at finite temperature T/ϵ_F as well as in the ground state. At large momenta k/k_F, we find that $n(k)$ falls off as C/k^4, in agreement with the Tan relations. From the asymptotics of $n(k)$, we determine the contact C as a function of T/ϵ_F and present a comparison with theory. At low T/ϵ_F, we find that C increases with temperature, and we tentatively identify a maximum around $T/\epsilon_F \simeq 0.4$. 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.

DOI: 10.1103/PhysRevLett.106.205302 PACS numbers: 67.85.De, 05.30.Fk, 67.10.Jn

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 [1] and its realization in ultracold atom experiments [2], the UFG has garnered widespread attention across multiple disciplines, including atomic physics [3], nuclear structure [4], and relativistic heavy-ion collisions [5]. 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:

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

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 interparticle distance $\sim k_F^{-1}$, without reference to the details of the interaction. While the thermodynamic properties of the UFG are *universal* [6], 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 [7] 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 rederived in multiple ways [8–10] as well as verified experimentally [11–13].

Recently, C has also been found to determine the prefactor of the high-frequency power-law decay of correlators [14,15], as well as the right-hand sides of the shear and bulk viscosity sum rules [15]. The contact is therefore a central piece of information on the UFG in equilibrium as well as away from equilibrium, since it constrains several thermodynamic quantities with a single number. On the experimental side, C has been shown to be central to radio-frequency spectroscopy and laser photoassociation [16], as well as to govern the rate of decrease of low-energy atoms due to inelastic two-body scattering processes with a large energy release. 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. [16].

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 [12]). One of the simplest relations concerns the asymptotics of the momentum distribution and asserts that

$$C \equiv \lim_{k\to\infty} k^4 n_\sigma(k), \qquad n_\sigma(k) \equiv \langle \hat{a}^\dagger_{\sigma,k} \hat{a}_{\sigma,k} \rangle, \tag{2}$$

where $n_\sigma(k)$ is the momentum distribution expressed as a thermal average and the $\hat{a}^\dagger_{\sigma,k}$ and $\hat{a}_{\sigma,k}$ denote creation and annihilation operators, respectively, for particles of momentum k and spin σ. If $n_\sigma(k)$ is normalized to the particle number N_σ, 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), by 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

$$\hat{H} \equiv \sum_k \frac{\hbar^2 k^2}{2m} (\hat{a}^\dagger_{\uparrow k} \hat{a}_{\uparrow k} + \hat{a}^\dagger_{\downarrow k} \hat{a}_{\downarrow k}) - g \sum_i \hat{n}_{\uparrow i} \hat{n}_{\downarrow i}, \tag{3}$$

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 σ at lattice position i. The equilibrium thermodynamical properties are obtained from the grand canonical partition function

$$\mathcal{Z} \equiv \mathrm{Tr}\exp[-\beta(\hat{H} - \mu\hat{N})], \tag{4}$$

where $\beta \equiv 1/k_B T$, μ is the chemical potential, and

$$\hat{N} \equiv \hat{N}_\uparrow + \hat{N}_\downarrow = \sum_i \hat{n}_{\uparrow i} + \sum_i \hat{n}_{\downarrow i} \tag{5}$$

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 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. (4), 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 $n \to 0$, respectively. The latter requires great care, as too low densities imply a departure from the thermodynamic limit. We find that $n \simeq 0.03$–0.05 particles per unit volume yield results accurate to $\simeq 7\%$ 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. First, we determine the bare lattice coupling constant g corresponding to the unitary regime by using Lüscher's formula [19] as in Ref. [20]. This procedure yields $g \simeq 5.14$ in the unitary limit. Second, we use the compact, continuous Hubbard-Stratonovich transformation

$$\exp(\tau g \hat{n}_{\uparrow i}\hat{n}_{\downarrow i}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\sigma_i [1 + B\sin(\sigma_i)\hat{n}_{\uparrow i}] \times [1 + B\sin(\sigma_i)\hat{n}_{\downarrow i}], \tag{6}$$

where σ_i (not to be confused with the spin projection) is the Hubbard-Stratonovich auxiliary field, with $B^2/2 \equiv \exp(\tau g) - 1$, and τ denotes the lattice spacing in the imaginary-time direction. We find that $\tau \simeq 0.05$ 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]. Third, we update the auxiliary field σ by using the hybrid Monte Carlo algorithm [23] (familiar from lattice QCD), which combines the Metropolis algorithm with deterministic molecular dynamics. Our implementation of the hybrid Monte Carlo 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 by 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/ϵ_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 ~200 uncorrelated auxiliary field samples for each data point give excellent statistics for $n(k)$. Multiplying $n(k)$ by k^4, as plotted in Fig. 2, we find a peak at $k \simeq k_F$ and a leveling out at high momenta, with the asymptotic regime setting in at $k \simeq 2k_F$ 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 $C/(Nk_F)$ as a function of T/ϵ_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 $k \simeq 4k_F$, 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. [24] by using density-density correlations, which yielded $C(T = 0)/(Nk_F) \simeq 3.4$, up to errors associated with fixing the nodes of the wave function. A more recent and comprehensive DMC calculation [25] came to the same conclusion by using the equation of state, the

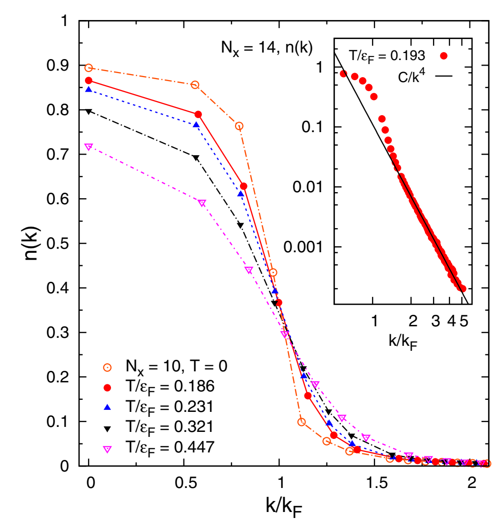

FIG. 1 (color online). Momentum distribution $n(k)$ from QMC calculations for $N_x = 10$ as a function of k/k_F, for various temperatures ranging from zero to $T/\epsilon_F \simeq 0.5$. The curves are intended as a guide to the eye, and the statistical errors are the size of the symbols. Inset: $n(k)$ for $N_x = 14$ in a log-log scale, showing the asymptotic $\sim k^{-4}$ behavior.

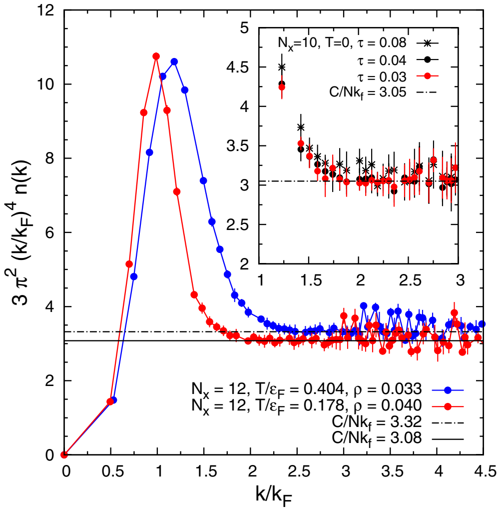

FIG. 2 (color online). Plot of $3\pi^2(k/k_F)^4 n(k)$ for $N_x = 12$ as a function of k/k_F at $T/\epsilon_F = 0.178$ and 0.404. The "plateaux" at large k/k_F give the (intensive) dimensionless quantity $C/(Nk_F)$. At low T/ϵ_F, the asymptotic region is reached at $k/k_F \simeq 2$. Inset: $N_x = 10$ results at $T = 0$ showing only slight dependence on the Suzuki-Trotter step τ.

momentum distribution, and the density-density correlation. In contrast, our present results indicate that $C(T = 0)/(Nk_F) \simeq 2.95 \pm 0.10$. 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

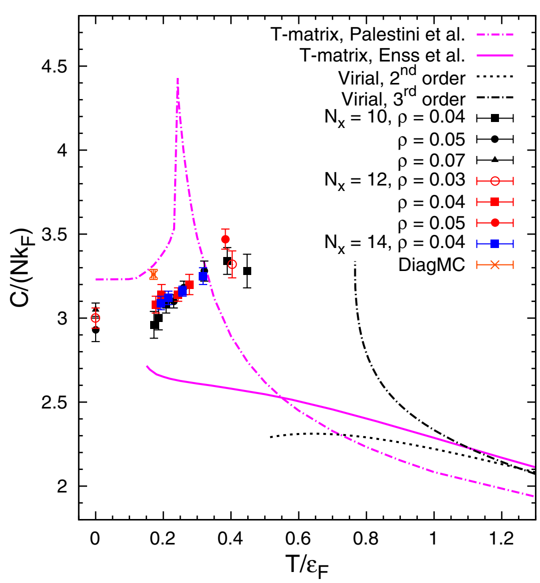

FIG. 3 (color online). Summary of QMC results for $C/(Nk_F)$ as a function of T/ϵ_F, as determined from the large k/k_F behavior of $n(k)$. The error bars are dominated by systematics related to the residual fluctuations in the plateaux, as exhibited in Fig. 2. Also shown are the t-matrix calculations of Refs. [27,28], the virial expansion of Ref. [29], and the diagrammatic Monte Carlo result of Ref. [34].

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/ϵ_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], which considered two different limits. At very low temperatures $T \ll T_c \simeq 0.15\epsilon_F$, 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 $C/(Nk_F) \simeq 16/3(\epsilon_F/T)$ 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 by using two different types of t-matrix approximations [27,28], as well as a third-order virial expansion [29]. 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. [29] 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 $C_{\max} \simeq 3.4$ at $T/\epsilon_F \simeq 0.4$. This scenario is in qualitative agreement with Ref. [26], 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 $C_{\max}$ 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 $k \simeq 2k_F$ at finite T/ϵ_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 wave function 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. 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/ϵ_F, by using the auxiliary field QMC method in conjunction with the hybrid Monte Carlo algorithm. While the ground-state momentum distribution was first determined via DMC calculations in Ref. [32], our results represent the first fully nonperturbative calculation of $n(k)$ free of uncontrolled approximations. We find that the contact at $T = 0$ assumes the value $\simeq 2.95 \pm 0.10$ and increases as a function of T/ϵ_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 $C/(Nk_F) \simeq 3.4$, while the analytic approach of Ref. [33], which interpolates smoothly between the strong- and weak-coupling limits, yields $C/(Nk_F) \simeq 3.0$, which is consistent with our data. Our results complement the calculations of Refs. [26–29] and are suggestive of a maximum in $C/(Nk_F)$ at $T/\epsilon_F \simeq 0.4$, which agrees qualitatively with Ref. [27] but disagrees with Ref. [28]. While calculations at higher $T/\epsilon_F \sim 1$ are feasible, an improved understanding of the finite density effects is clearly called for.

We thank R.J. Furnstahl for encouragement and A. Bulgac, J. Carlson, S. Gandolfi, A. Gezerlis, and K. Schmidt for instructive discussions and comments. We are also grateful to T. Enss, H. Hu, and F. Palestini for giving us access to their respective results. We acknowledge support under U.S. DOE Grants No. DE-FG02-00ER41132 and No. DE-AC02-05CH11231, UNEDF SciDAC Collaboration Grant No. DE-FC02-09ER41586, and NSF Grant No. PHY-0653312. This study was supported, in part, by the Academy of Finland through its Centers of Excellence Program (2006–2011), the Vilho, Yrjö, and Kalle Väisälä Foundation of the Finnish Academy of Science and Letters, and the Waldemar von Frenckell and Magnus Ehrnrooth Foundations of the Finnish Society of Sciences and Letters. Part of this work was performed by using an allocation of computing time from the Ohio Supercomputer Center.

[1] ''The Many-Body Challenge Problem,'' formulated by G.F. Bertsch (1999); see, e.g., *Recent Progress in Many-Body Theories*, Series on Advances in Quantum Many-Body Theory Vol. 3, edited by R. F. Bishop, K. A. Gernoth, N.R. Walet, and Y. Xian (World Scientific, Singapore, 2000).

[2] K.M. O'Hara *et al.*, Science **298**, 2179 (2002); T. Bourdel *et al.*, Phys. Rev. Lett. **91**, 020402 (2003); C.A. Regal *et al.*, Nature (London) **424**, 47 (2003); K.E. Strecker, G.B. Partridge, and R.G. Hulet, Phys. Rev. Lett. **91**, 080406 (2003); J. Cubizolles *et al.*, *ibid.* **91**, 240401 (2003); S. Jochim *et al.*, *ibid.* **91**, 240402 (2003); K. Dieckmann *et al.*, *ibid.* **89**, 203201 (2002).

[3] S. Giorgini, L.P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 2008); I. Bloch, J. Dalibard, W. Zwerger, *ibid.* **80**, 885 (2008).

[4] C.J. Pethick and D.G. Ravenhall, Annu. Rev. Nucl. Part. Sci. **45**, 429 (1995); J. Carlson *et al.*, Phys. Rev. C **68**, 025802 (2003); C.J. Horowitz and A. Schwenk, Phys. Lett. B **638**, 153 (2006).

[5] T. Schäfer, Physics **2**, 88 (2009); T. Schäfer and D. Teaney, Rep. Prog. Phys. **72**, 126001 (2009).

[6] H. Heiselberg, Phys. Rev. A **63**, 043606 (2001); T.-L. Ho, Phys. Rev. Lett. **92**, 090402 (2004).

[7] S. Tan, Ann. Phys. (N.Y.) **323**, 2952 (2008); **323**, 2971 (2008); **323**, 2987 (2008).

[8] S. Zhang and A.J. Leggett, Phys. Rev. A **77**, 033614 (2008).

[9] F. Werner, Phys. Rev. A **78**, 025601 (2008).

[10] E. Braaten and L. Platter, Phys. Rev. Lett. **100**, 205301 (2008); E. Braaten, D. Kang, and L. Platter, *ibid.* **104**, 223004 (2010).

[11] J.E. Thomas, J. Kinast, and A. Turlapov, Phys. Rev. Lett. **95**, 120402 (2005).

[12] J.T. Stewart *et al.*, Phys. Rev. Lett. **104**, 235301 (2010); D.E. Sheehy, Physics **3**, 48 (2010).

[13] E.D. Kuhnle *et al.*, Phys. Rev. Lett. **105**, 070402 (2010).

[14] D.T. Son and E.G. Thompson, Phys. Rev. A **81**, 063634 (2010).

[15] E. Taylor and M. Randeria, Phys. Rev. A **81**, 053610 (2010).

[16] E. Braaten, arXiv:1008.2922.

[17] R.L. Stratonovich, Sov. Phys. Dokl. **2**, 416 (1958); J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959).

[18] A. Bulgac, J.E. Drut, P. Magierski, Phys. Rev. Lett. **96**, 090404 (2006); Phys. Rev. A **78**, 023625 (2008).

[19] M. Lüscher, Commun. Math. Phys. **105**, 153 (1986).

[20] D. Lee and T. Schäfer, Phys. Rev. C **73**, 015201 (2006); **73**, 015202 (2006).

[21] D. Lee, Phys. Rev. C **78**, 024001 (2008); Prog. Part. Nucl. Phys. **63**, 117 (2009).

[22] J.E. Hirsch, Phys. Rev. B **28**, R4059 (1983).

[23] S. Duane *et al.*, Phys. Lett. B **195**, 216 (1987); S.A. Gottlieb *et al.*, Phys. Rev. D **35**, 2531 (1987).

[24] R. Combescot, S. Giorgini, and S. Stringari, Europhys. Lett. **75**, 695 (2006); C. Lobo *et al.*, Phys. Rev. Lett. **97**, 100405 (2006).

[25] S. Gandolfi, K.E. Schmidt, and J. Carlson, Phys. Rev. A **83**, 041601(R) (2011).

[26] Z. Yu, G.M. Bruun, and G. Baym, Phys. Rev. A **80**, 023615 (2009).

[27] F. Palestini *et al.*, Phys. Rev. A **82**, 021605(R) (2010).

[28] T. Enss, R. Haussmann, and W. Zwerger, Ann. Phys. (N.Y.) **326**, 770 (2011).

[29] H. Hu, X.-J. Liu, and P. Drummond, New J. Phys. **13**, 035007 (2011).

[30] J.T. Stewart, J.P. Gaebler, and D.S. Jin, Nature (London) **454**, 744 (2008); P. Magierski *et al.*, Phys. Rev. Lett. **103**, 210403 (2009); J.P. Gaebler *et al.*, Nature Phys. **6**, 569 (2010).

[31] E.D. Kuhnle *et al.*, Phys. Rev. Lett. **106**, 170402 (2011).

[32] G.E. Astrakharchik *et al.*, Phys. Rev. Lett. **95**, 230405 (2005); A.J. Morris, P. López Ríos, and R.J. Needs, Phys. Rev. A **81**, 033619 (2010).

[33] R. Haussmann, M. Punk, and W. Zwerger, Phys. Rev. A **80**, 063612 (2009).

[34] O. Goulko and M. Wingate, Proc. Sci., Lattice2010 (2010) 187.