Emergence of a pseudogap in the BCS–BEC crossover

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(Dated: August 12, 2020)

Strongly correlated Fermi systems with pairing interactions become superfluid below a critical temperature $T_c$. The extent to which such pairing correlations alter the behavior of the liquid at temperatures $T > T_c$ is a subtle issue that remains an area of debate, in particular regarding the appearance of the so-called pseudogap in the BCS–BEC crossover of unpolarized spin-1/2 nonrelativistic matter. To shed light on this, we extract several quantities of crucial importance at and around the unitary limit, namely: the odd-even staggering of the total energy, the spin susceptibility, the pairing correlation function, the condensate fraction, and the critical temperature $T_c$, using a non-perturbative, constrained-ensemble quantum Monte Carlo algorithm.

Introduction. Dilute, two-component Fermi gases with short-range interactions are relevant to a variety of systems in nuclear and condensed matter physics [1, 2]. In ultracold atomic gases [3, 4], the strength of the interaction can be tuned essentially at will by driving the system across a Feshbach resonance using an external magnetic field [5], from a weakly coupled state, well-described by Bardeen, Cooper, Schrieffer (BCS) theory, to a state with molecular bound states corresponding to a Bose-Einstein Condensate (BEC). A smooth crossover [1, 6] links these limiting regimes as one changes the sign of the Einstein field [5], from a weakly coupled state, well-described by previously employed projection for the total particle number, we introduce a new projection for the particle number asymmetry only, which is free of the infamous sign problem [11]. We simulate on a cubic lattice of size $L = N_x \ell$, set units such that $\hbar = k_B = m = 1$, and set the spatial lattice spacing to $\ell = 1$, which is equivalent to a choice of “lattice units.” $N_x$ therefore dictates the lattice size and approach to the thermodynamic limit. We use $N$ to denote the total particle number, $N = N_\uparrow + N_\downarrow$, where $N_\sigma$ is the number of spin-$\sigma$ particles with $\sigma \in \{\uparrow, \downarrow\}$, not to be confused with the particle number asymmetry $N_- = N_\uparrow - N_\downarrow$. 

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arXiv:2004.05014v3 [cond-mat.quant-gas] 11 Aug 2020
FIG. 1. Left: The condensate fraction $\alpha$ as a function of temperature at different scattering lengths; at a fixed temperature, $\alpha$ increases toward the BEC limit. At all scattering lengths, the condensate fraction tends to decrease with an increase in lattice size. At $1/(k_F a) = 0.2$, Astrakharchik et al. [12] estimated the zero-temperature condensate fraction as $\alpha(T = 0) \approx 0.65$. Right (top): characteristic temperatures in the BCS–BEC crossover; $T_c$ is the superfluid critical temperature; $T_s$ is a lower bound on the temperature at which the spin susceptibility peaks; and $T^*$ is the temperature at which the pairing gap disappears. Our estimate for $T_c$ agrees with the experimental value from Ku et al. [13]. Right (bottom): $\alpha$ at unitarity; error bars for our results are typically within the marker size. Also shown: the experimental results of Ku et al. [13], Sanner et al. [15], and the previous AFQMC studies of Bulgac et al. [16] (BDM) and Jensen et al. [16] (JGA). We also plot zero-temperature results by Astrakharchik et al. [12] (ABCG) and He et al. [17] (HLLL). The large condensate fraction measured by Sanner et al. is relevant to our comparison of the spin susceptibility in Fig. 2. The JGA estimates, derived from the maximum eigenvalue of the two-body density matrix, are closer to the experimental results especially at high temperature, whereas the finite-size scaling of our results, derived from the asymptotic values of $h(k_F r)$, yields more accurate estimates of the critical temperature $T_c$. The discrepancy between our results and BDM, which are also derived from the asymptotic behavior of $h(k_F r)$, support the argument of Jensen et al. [16] that the difference is due to the BDM spherical momentum cutoff. $T_c$ estimates are compatible with previous estimates by Burovski et al. [18] and Bulgac et al. [15]. Estimates for $T^*$ are compatible with previous results by Magierski et al. [19].

**Results.** We determined the condensate fraction, critical temperature, spin susceptibility, even-odd pairing gap, and energy per particle. We also performed the first finite-temperature measurements of the Tan contact away from unitarity. Given the ongoing debate over pseudogap signatures and the relationship between the Tan contact, which is dominated by short-range interaction effects, and pairing, which characterizes long-range correlations (see Refs. [7, 20]), we defer these results to the supplementary material [9]. Error bars on individual points represent statistical errors and show the standard error of the mean. Error bars in Figs. 3 and 4 incorporate statistical errors and finite volume effects and represent the standard error of the mean.

(i) **Condensate fraction:** The condensate fraction can be obtained from the asymptotic behavior of the quantity $h(r)$ [12, 15, 18]:

$$\alpha = \lim_{r \to \infty} h(r), \quad h(r) = \frac{N}{2} \left( g_2(r) - g_1(r) r^2 \right), \quad (1)$$

$$g_2(r) = \left( \frac{3}{\pi} \right)^2 \int d^3 r_1 d^3 r_2 \left( \psi_1^\dagger (r_1) \psi_1^\dagger (r_2) \psi_1 (r_2) \psi_1 (r_1) \right),$$

$$g_1(r) = \frac{2}{N} \int d^3 r_1 \left( \psi_1^\dagger (r_1) \psi_1 (r_1) \right), \quad r_{1,2} \equiv r_{1,2} + r,$$

which acts as an order parameter, characterizing the extent of off-diagonal long-range order [21]. In Fig. 1, we show our results for $\alpha$ at different scattering lengths. An alternative approach is to estimate $\alpha$ as the maximum eigenvalue of $g_2$ [22]. Comparing our results to those of the eigenvalue method, and to experimental values in the right panel of Fig. 1, suggests that the eigenvalue method approaches the experimental $\alpha$ more quickly than our asymptotic value method, most noticeably at higher $T$.

However, we also use the finite-size scaling of $\alpha$ to
determine $T_c$. By calculating $\alpha$ at multiple temperatures and lattice sizes, we obtain “crossing temperatures” (i.e., lattice-size-dependent estimates of $T_c$) from which we extrapolate to infinite volume to determine the true $T_c$ [9, 12, 15, 18]. That procedure yields $T_c$ as shown in Fig. 1, which are consistent with previous studies [15, 18] and in agreement with the experimental result $T_c/\varepsilon_F = 0.167(13)$ at unitarity [13].

(ii) Spin susceptibility: A probe of the normal state character of the pairing is the spin-susceptibility $\chi_s$, which should be suppressed below $T^*$, as fermions bind into pairs, making the gas strongly diamagnetic [26]. This is also naturally related to the fluctuations in particle asymmetry by

$$\chi_s = \frac{1}{TV} \langle \hat{N}_s^2 \rangle = \frac{1}{TV} \left( \langle \hat{N}_\uparrow - \hat{N}_\downarrow \rangle^2 \right).$$

In Fig. 2, we show our results for $\chi_s$. We use the particle-asymmetry constrained ensemble, which is completely sign-problem free [9]. Our results demonstrate an expected decrease in the maximal value of $\chi_s$ as $1/(k_F a)$ increases toward the BEC regime. We also find a moderate suppression of $\chi_s$ above $T_c$, which increases towards the BEC regime. In the lower panel of Fig. 2, we compare our results at unitarity to two previous AFQMC calculations [22, 23], an estimate using strong-coupling Luttinger-Ward theory [24], an experimental result from Sanner et al. [14], the prediction from normal Fermi liquid theory (nFLT), and a self-consistent NSR estimate from Pantel et al. [25]. The deviation from FLT behavior confirms symmetry-based arguments by Rothstein and Shrivastava [27] that 3D unitary Fermi gases cannot be adequately described by nFLT in the range $T_c < T < T_F$. Our suppression in $\chi_s$ is less severe than in calculations by Wlazłowski et al. [23], supporting the argument by Jensen et al. [22] that said suppression is affected by the choice of spherical cutoff. The experimental value is suppressed due to their finite condensate fraction even above $T_c$, which can be seen in Fig. 1. However, our spin susceptibility is more suppressed than in both Jensen et al. and Enss and Haussmann [24], and, more importantly, the effect seems to grow for larger systems rather than lessen. Figure 2 also shows our results for the spin susceptibility for $0.1 \leq 1/(k_F a) \leq 0.3$. To our knowledge, these are the first QMC measurements of $\chi_s$ away from unitarity.

Tajima et al. [28, 29] identified the temperature at which $\chi_s$ peaks as $T_s$, and the temperature range $T_c < T < T_s$ as the “spin-gap” range where there are fewer free spins to contribute to $\chi_s$. Although they find that $T_s \sim T^*$, the exact relationship between these two temperatures requires further study. We present only lower bounds for the temperature $T_s$ in Fig. 1.

(iii) Energy stagger pairing gap: The even-odd staggering of systems with fixed particle numbers has been used as a measure of pairing since early studies of nuclear structure [30]. On the other hand, the physical origin of the pseudogap, and consequently the way one should measure it, has been the core of a long debate since the early days of high-Tc superconductivity (see Randeria [31] for a review). It should be noted that our use of the even-odd staggering gap as a measure of the pseudogap presupposes that the pseudogap origin lies in the preformation of Cooper pairs above $T_c$. Several finite-difference formulas have been used to circumvent this (see Ref [32] for in-depth discussions). The simplest one is the three-point estimate, $\Delta_E^{(3)}$, which assumes a linear equation of state. If the equation of state has positive curvature, $\Delta_E^{(3)}$ will underestimate the pairing gap when $N$ is even and overestimate the pairing gap when $N$ is odd. Instead, we use the five-point expression

$$\Delta_E^{(5)} = \frac{(-1)^N}{8} \sum_{s=\pm 1} \left[ 4E(N+s) - E(N+2s) - 3E(N) \right].$$
where $E(N)$ is the ground state energy of a system with $N$ total particles, which will be achieved when $|N_-| = \text{mod}(N, 2)$. In addition to calculating $\Delta_E^{(5)}$, we propose another estimation method, which is to fit the energies calculated for many different values of $N$ and $N_-$ to a two-parameter equation of state,

$$
\frac{E}{E_{FG}}(\xi, \Delta_E^{(f)}) = \xi + |N_-| \frac{\Delta_E^{(f)}}{E_{FG}},
$$

\hspace{1cm} (4)

where $\xi(T/\varepsilon_F, 1/(k_F a))$ is a temperature-dependent generalization of the Bertsch parameter, $\varepsilon_F = (\hbar^2 k_F^2) / (2m)$ is the Fermi energy, $E_{FG} = 3N\varepsilon_F / 5$ is the energy of a free Fermi gas at zero-temperature, and we use $|N_-| \in \{0, 1, 2\}$ for the fitting procedure [9]. Regardless of the estimation scheme, we expect $\Delta_E$ to become finite below some temperature $T^\ast$. If $T^\ast$ exceeds the critical temperature $T_c$, this garners support for the existence of a pseudogap.

In Fig. 3, we present our results for the even-odd pairing gap, derived from both $\Delta_E^{(5)}$ and $\Delta_E^{(f)}$ [9]. Our method for calculating both the pairing gap and the energy equation of state produces a profusion of data points, making visual comparison difficult. We therefore plot the results of a regression that includes all lattice sizes with $N_x \geq 8$, with further details provided in the supplementary material [9]. In the lower panel, we compare our results at unitarity to previous theoretical and experimental studies: an AFQMC measurement of the spectral gap which employed a spherical momentum cutoff (MWB, [19]); a constrained ensemble AFQMC study (JGA, [22]) that estimated $\Delta_E^{(5)}$ with a cubic cutoff, but without relative temperature corrections, which we discuss in the supplement [9]; two low-temperature experimental results [34, 35]; and a zero-temperature QMC reference result [33]. We can view our results as charting a middle course between the Jensen et al. results and the Magierski et al. results, all of which can be interpreted as approaching the low-temperature reference results. However, the comparison is fraught since the spectral gap computed by Magierski et al. [19] is a priori a different quantity than the even-odd pairing gap and the critical temperature computed by Jensen et al. is lower than ours and also the experimentally determined value.

Despite the large uncertainties at low temperatures, we can appreciate certain features of the pairing gap. It is weaker, compared to the low temperature limit, for temperatures above $T_c$, however, it cannot be said to vanish immediately above the $T_c$ error band even at unitarity. Our estimates for $T^\ast$, derived from spline fits [9] of both $\Delta_E^{(5)}$, see Eq. (3), and $\Delta_E^{(f)}$, see Eq. (4), are presented in Fig. 1 and are comparable with a previous AFQMC study that determined $T^\ast$ from the spectral gap [19], as opposed to the even-odd energy gap [22]. At $1/(k_F a) \approx 0.3$, we detect a plateau in the pairing gap above $T_c$. At this scattering length, $na^3 \sim 1$ so that the interparticle separation is of the same scale as the Cooper pair size, indicating a crossing into the “pure” BEC regime, where the pseudogap maintains a plateau to very high temperatures.

(iv) Energy equation of state: Equation (4), which parameterizes the energies of systems with various numbers of $N_{\uparrow \downarrow}$, also allows us to extract the temperature- and coupling constant-dependent Bertsch parameter $\xi(T/\varepsilon_F, 1/(k_F a))$. In Fig. 4 we show our results for $\xi(T/\varepsilon_F, 1/(k_F a))$ for each scattering length and compare to previous results. Similar to the results by Drut et al. [36] at unitarity, we did not capture the curvature in the equation of state seen by Ku et al. [13] below $T_c$. However, our results at unitarity do approach the reference values at zero temperature. We have a similar level of agreement with the results of Van Houcke et al. [39], which are not shown in Fig. 4, but are in excellent agreement with experiment in the normal state. We provide a table of values and errors for both $\xi$ and $\Delta$.
FIG. 4. AFQMC results for the temperature-dependent Bertsch parameter, \( \xi(T/\varepsilon_F, 1/(k_F a)) \) at four different scattering lengths. We incorporate results for all lattices with \( N_z \geq 8 \) using a regression technique described in the supplemental material [9]. At unitarity, we compare our results to the experimental measurements of Ku et al. [13] and the high-precision AFQMC results of Drut et al. [36] (DLWM). We also show the zero temperature predictions of Carlson et al. [37] (CGSZ) at unitarity and of Astrakharchik et al. [38] (ABCG) at all scattering lengths.

in the supplemental material [9].

Conclusion. We performed the first ab initio finite-temperature calculations of the spin susceptibility \( \chi_s \) and Tan contact \( C \) away from unitarity, in addition to determining the condensate fraction \( \alpha \), the critical temperature \( T_c \), the even-odd pairing gap \( \Delta_E \), and the Bertsch parameter \( \xi \). For both the spin susceptibility and the even-odd pairing gap, we find no discontinuities as we reduce the coupling, but rather a smooth reduction in pseudogap signatures.

Since the BCS–BEC crossover is smooth, we do not expect an abrupt and discontinuous emergence of the pseudogap. Questions about where the pseudogap emerges are therefore analogous to long-debated questions about where the Earth’s atmosphere ends [40]. Since the field is young, we have not yet developed the pseudogap analog of the Kármán line from space science. We have provided context to this discussion by looking for signatures of the pseudogap between 0.0 \( \leq 1/(k_F a) \leq 0.3 \). At 1/(\( k_F a \) = 0.3, we see strong pseudogap signatures, which diminish towards unitarity. However, all characteristic temperatures \( T^* \) in Fig. 1 exceed the critical temperature \( T_c \) at all scattering lengths. Based on our results, we conclude it is premature to exclude unitarity from the pseudogap regime. Future work should include more refined extrapolations to the limit of zero-effective range, infinite volume, and zero density.

Acknowledgments.- We thank G. Wlazlowski for his valuable input and K. Roche and S. Jin for their guidance on the computational implementation. ARH and AB were supported by U.S. Department of Energy, Office of Science, Grant No. DE-FG02-97ER41014. ARH was also supported by the U.S. Department of Energy, Computational Science Graduate Fellowship, under Grant No. DE-FG02-97ER2508. JD was supported by the U.S. National Science Foundation under Grant No. PHY1452635. This research used resources of the Oak Ridge Leadership Computing Facility, which is a US DOE Office of Science User facility supported under Contract No. DE-AC05-00OR22725. This work was supported by “High Performance Computing Infrastructure” in Japan, Project ID: hp180048. A series of simulations were carried out on the Tsubame 3.0 supercomputer at Tokyo Institute of Technology. It was also facilitated through the use of advanced computational, storage, and networking infrastructure provided by the Hyak supercomputer system and funded by the STF at the University of Washington.

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