PHYSICAL REVIEW A **77**, 061605(R) (2008)

Comparative study of strong-coupling theories of a trapped Fermi gas at unitarity

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(Received 4 December 2007; published 27 June 2008)

We present a systematic comparison of the most recent thermodynamic measurements of a trapped Fermi gas at unitarity with predictions from strong-coupling theories and quantum Monte Carlo (MC) simulations. The accuracy of the experimental data, of the order of a few percent, allows a precise test of different many-body approaches. We find that a Nozières and Schmitt-Rink treatment of fluctuations is in excellent agreement with the experimental data and available MC calculations at unitarity.

DOI: 10.1103/PhysRevA.77.061605 PACS number(s): 03.75.Hh, 03.75.Ss, 05.30.Fk

The theory of strongly interacting fermions is of great interest. Interacting fermions are involved in some of the most important unanswered questions in condensed matter physics, nuclear physics, astrophysics, and cosmology. Though weakly interacting fermions are well understood, new approaches are required to treat strong interactions. In these cases, one encounters a "strongly correlated" picture which occurs in many fundamental systems ranging from strongly interacting electrons to quarks.

The main theoretical difficulty lies in the absence of any small coupling parameter in the strongly interacting regime, which is crucial for estimating the errors of approximate approaches. Although there are numerous efforts to develop strong-coupling perturbation theories of interacting fermions, notably the many-body T-matrix fluctuation theories [1–10], their accuracy is not well understood. Quantum Monte Carlo (QMC) simulations are also less helpful than one would like, due to the sign problem for fermions [11] or, in the case of lattice calculations [12,13], the need for extrapolation to the zero filling factor limit.

Recent developments in ultracold atomic Fermi gases near a Feshbach resonance with widely tunable interaction strength, densities, and temperatures have provided a unique opportunity to *quantitatively* test different strong-coupling theories [14–18]. In these systems, when tuned to have an infinite s-wave scattering length—the *unitarity* limit—a simple universal thermodynamic behavior emerges [19,20]. Due to the pioneering efforts of many experimentalists, the accuracy of thermodynamic measurements at unitarity has improved significantly. A breakthrough occurred in early 2007, when both energy and entropy in trapped Fermi gases were measured without invoking any specific theoretical model [18]. This milestone experiment, arguably the most accurate measurement in cold atoms, has an accuracy at the level of a few percent.

In this Rapid Communication, using experimental data as a benchmark, we present an *unbiased* test of several strong-coupling theories that are commonly used in the literature, including QMC simulations. From this comparison, we show that the simplest theory which incorporates pairing fluctuations appears to be *quantitatively* accurate at unitarity. This is the T-matrix approximation pioneered by Nozières and Schmitt-Rink (NSR) [1] and others [2,5], as recently applied to trapped gases in the below threshold superfluid regime [8]. We find it describes the observed thermodynamics extremely well at all temperatures at unitarity, except in regions very near the superfluid transition temperature T_c.

The comparisons show that the simple NSR approximation gives excellent results. This appears to be related to the important symmetry property of scale invariance [21], which is a necessary feature of any exact theory at unitarity, and is shared by the NSR approach. Our comparative results should therefore be useful in developing theoretical approaches for strong interacting fermions, and are relevant to many fields of physics. In particular, our results might shed light on the applicability of different T-matrix approximations to high-T_c superconductors and neutron stars, which are of interest to the condensed matter and astrophysics communities.

The strong-coupling theories that we compare include several T-matrix fluctuation and QMC theories. We refer to Refs. [12,13] for a detailed description of QMC methods, and briefly review different T-matrix theories. These involve an infinite set of diagrams—the ladder sum in the particle-particle channel. It is generally accepted that this ladder sum is necessary for taking into account strong pair fluctuations in the strongly interacting regime, since it is the leading class of all sets of diagrams [22].

The diagrammatic *structure* of different T-matrix theories may be clarified *above* T_c for a single-channel model [7], where one writes for the T matrix, $t(Q)=U/[1+U\chi(Q)]$. Here and throughout, $Q=(\mathbf{q},i\nu_n)$, $K=(\mathbf{k},i\omega_m)$, while $U^{-1}=m/(4\pi\hbar^2 a)-\Sigma_{\mathbf{k}} m/\hbar^2\mathbf{k}^2$ is the bare contact interaction expressed in terms of the s-wave scattering length. We use $\Sigma_K=k_BT\Sigma_m\Sigma_{\mathbf{k}}$, where $\mathbf{q}$ and $\mathbf{k}$ are wave vectors, while ν_n and ω_m are bosonic and fermionic Matsubara frequencies.

Different T-matrix fluctuation theories differ in their choice of the particle-particle propagator [22]

$$\chi(Q)=\sum_K G_\alpha(K)G_\beta(Q-K), \tag{1}$$

and the associated self-energy, $\Sigma(K)=\Sigma_Q t(Q)G_\gamma(Q-K)$. The subscripts α, β, and γ in the above equations can either be set to "0," indicating a noninteracting Green's function $G_0(K)=1/[i\omega_m-\hbar^2\mathbf{k}^2/2m+\mu]$, or be absent, indicating a fully dressed interacting Green's function. In these cases a Dyson equation, $G(K)=G_0(K)/[1-G_0(K)\Sigma(K)]$, is required to self-consistently determine G and Σ. The only free param-

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eter, the chemical potential μ, is fixed by the number equation, $N=2\Sigma_K G(K)$.

By taking different combinations of α, β, and γ, there are six distinct choices of the T-matrix approximation, for which a nomenclature of $(G_\alpha G_\beta)G_\gamma$ will be used. As noted earlier, there is no known *a priori* theoretical justification for which is the most appropriate. While having the same diagrammatic structure, the T-matrix approximations we use above and below T_c are computationally different, owing to the use of different G_0 (or G). Below T_c, these Green's functions are 2×2 matrices.

The simplest choice, $(G_0G_0)G_0$, was pioneered by NSR above T_c using the thermodynamic potential [1], with a truncated Dyson equation for G, i.e., $G=G_0+G_0\Sigma G_0$. This theory was extended to the broken-symmetry superfluid phase by several authors [4,5,8,23], using the mean-field 2×2 matrix BCS Green's function as "G_0." In Ref. [8], it was shown that the resulting ground state energy is in excellent agreement with the zero-temperature QMC calculation for all interaction strengths. The NSR approximation is the simplest scheme that includes the effects of particle-particle fluctuations. It does not attempt to be self-consistent. In the other extreme, one may consider a $(GG)G$ approximation, with a fully self-consistent propagator. This was investigated in detail by Haussmann *et al.*, both above [3] and below T_c [10]. Below T_c an *ad hoc* renormalization of the interaction strength is required to obtain a gapless phonon spectrum.

We also consider an intermediate scheme having an asymmetric form for the particle-particle propagator, i.e., $(GG_0)G_0$. This has been discussed in a series of papers by Chen *et al.* [7], based on the assumption that this treatment of fluctuations is consistent with the simpler BCS theory at low temperatures. Although the theory has been explored numerically to some extent [24], a complete numerical solution has not been implemented previously. A simplified version [7] of the $(GG_0)G_0$ fluctuation theory was introduced based on a decomposition of the T-matrix $t(Q)$ in terms of a condensate part and a pseudogap part. In this Rapid Communication, we refer to this approach as the "pseudogap model" and will include it in our comparative study.

Other strong-coupling theories with an *artificial* small parameter have been developed recently, including an ϵ expansion around the critical dimension [25] and a $1/N$ expansion for a $2N$-component gas [26]. These field-theoretic approaches provide very useful but so far only qualitative information about universal thermodynamics valid at unitarity. In the Boltzmann regime at high temperatures, not explored experimentally so far, it is possible to make a *virial* expansion in terms of fugacity [27]. We have verified that the three T-matrix schemes we study here do correctly include the dominant second-order virial contribution in the high-temperature region.

Figure 1 compares the temperature dependence of the chemical potential at unitarity, calculated from different T-matrix schemes and lattice QMC simulations. The T-matrix approximations above T_c have been solved using an adaptive step Fourier transform method. Below T_c, the NSR and $(GG)G$ results are from Refs. [8,10], respectively. The $(GG_0)G_0$ approximation below T_c has not been worked out yet. The QMC results are taken from Refs. [12,13]. However,

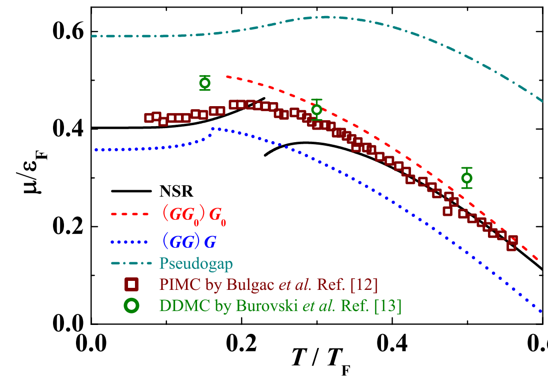

FIG. 1. (Color online) Chemical potential of a uniform Fermi gas at unitarity as a function of reduced temperature T/T_F, where $T_F=\epsilon_F/k_B$. The lines plotted are the results of NSR (solid lines), $(GG_0)G_0$ (dashed line), $(GG)G$ (dotted line), and pesudogap model (dotted-dashed line). These predictions are compared with lattice QMC simulations (symbols).

these lattice calculations may have systematic errors due to an extrapolation to the zero filling factor limit which is necessary to have a well-defined continuum theory. Nonetheless, the three T-matrix calculations agree well with the lattice QMC simulations. On the other hand, the prediction of the pesudogap model above T_c differs substantially from the $(GG_0)G_0$ results, for which it is an approximation. The pseudogap model omits important features of the full $(GG_0)G_0$ theory, due to the "condensate" + "pseudogap" decomposition of the T matrix.

The determination of energy and entropy is a subtle problem. It is known that universal thermodynamics at unitarity implies a rigorous scaling relation [19], $P=-\Omega=2E/3$, which relates the pressure (or thermodynamic potential) and the energy density for a unitarity gas in the same way as for an ideal, noninteracting quantum gas, although the energy densities are quite different. Apart from the $(GG)G$ scheme above T_c and the NSR approach (in both regimes), strong-coupling theories in general *do not* satisfy this essential scaling relation. The violation is typically at the level of a few percent, comparable to the accuracy of the experimental data we used. For quantitative purposes, we calculate the thermodynamic potential from the chemical potential, using

$$\Omega(\mu,T=\text{const}) = -\int_{\mu_0}^{\mu} n(\mu')d\mu' + \Omega(\mu_0,T) \qquad (2)$$

at a given temperature. Here, the lower bound of the integral μ_0 is sufficiently small so that $\Omega(\mu_0,T)$ can be obtained accurately from a high-temperature virial expansion [27]. The energy and entropy can then be calculated from the rigorous scaling relations, $E=-3\Omega/2$, and $S=(-5\Omega/2-\mu N)/T$, valid at unitarity.

The energy and entropy obtained in this manner are given in Fig. 2, and compared to the predictions of QMC calculations. There is a reasonable agreement between T-matrix theories and the lattice QMC simulations. For the energy, we also show the path-integral Monte Carlo results of Akkineni *et al.* for the *continuum* model [11]. At temperatures above

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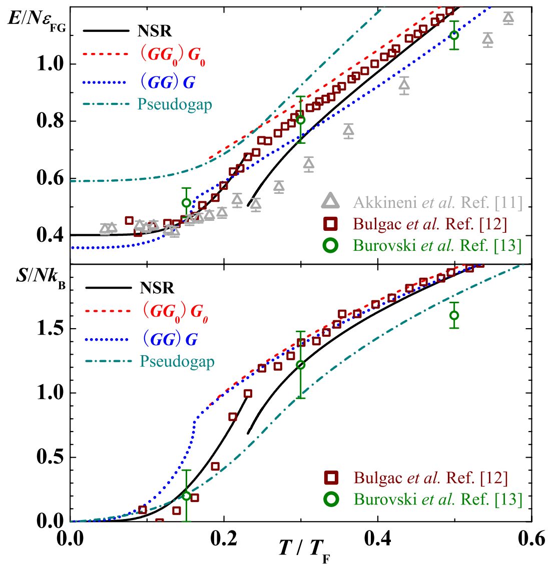

FIG. 2. (Color online) Temperature dependence of the energy (upper panel) and of the entropy (lower panel) of a uniform Fermi gas at unitarity, obtained from different T-matrix approximations and QMC simulations as indicated.

$0.2T_F$, the energy lies systematically below that of all the T-matrix theories. This is probably due to the use of a finite effective range r_0 for the interaction [11], i.e., $k_F r_0 \simeq 0.3$. Compared to the QMC results, the pseudogap model appears to provide the least accurate predictions for energy and entropy. At low temperatures it predicts a $T^{3/2}$ dependence for the entropy, which is characteristic of a noninteracting ideal Bose condensed gas. In contrast, the T-matrix entropies follow a T^3 scaling law, arising from the Bogoliubov-Anderson phonon modes [10].

We now compare theoretical predictions with experimental data [18]. A strongly interacting Fermi gas of $N=1.3(2)\times 10^5$ lithium atoms is prepared in a Gaussian trap $V(\mathbf{r})=V_0\{1-\exp[-m(\omega_\perp^2\rho^2+\omega_z^2 z^2)/(2V_0)]\}$ with $V_0\simeq 10E_F$ at a magnetic field $B=840$ G, slightly above the resonance position $B_0=834$ G. The large but finite interaction, $k_F a=-20.0$, leads to an approximately 1% correction that is not accounted for experimentally. The energy is determined in a model-independent way from the mean square radius $\langle z^2\rangle$ of the strongly interacting cloud, according to the virial theorem, which states that the potential energy ($\propto\langle z^2\rangle$) of the gas is a half of its total energy. The entropy of the gas is calibrated again from the cloud size, but after an adiabatic sweep to a weakly interacting gas with $k_F a=-0.75$, using a precise theory at weak coupling. We refer to Refs. [18,20] for further details. To determine the energy and entropy theoretically, we apply the local density approximation by assuming that the system can be treated as locally uniform, with a position-dependent local chemical potential $\mu_{\text{hom}}[n(\mathbf{r}),T/T_F(n)]=\mu-V(\mathbf{r})$, where $T_F(n)$ is the local Fermi temperature. From this condition, the density profile is obtained, and the total energy and entropy are calculated.

Figure 3 shows the interaction energy vs entropy in a harmonic trap as predicted by the strong-coupling theories in comparison with experimental data. All results of perturbation theories, except that of the NSR approach, were not reported previously to our knowledge. The energy is expressed in units of the Fermi energy at zero temperature in a harmonic trap: $E_F=(3N\omega_\perp^2\omega_z)^{1/3}=k_B T_F$. To emphasize the effects of interactions, we have subtracted the ideal gas result E_{IG}. No adjustable parameters have been used theoretically or experimentally. This comparison is therefore an unbiased test of how well T-matrix theories agree with experiment [18].

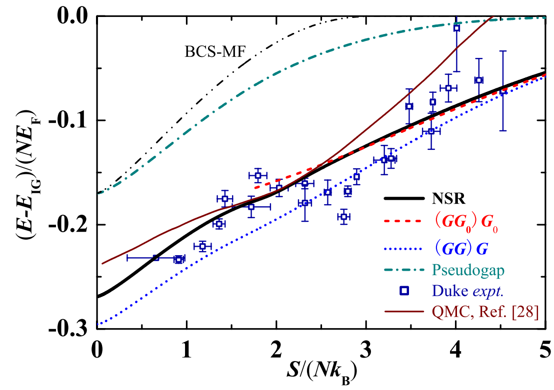

FIG. 3. (Color online) Theoretically predicted universal thermodynamics in comparison with experimental data [18].

The difference between different T-matrix schemes, mostly of the order $0.05NE_F$, is relatively small and thus nearly indistinguishable in the plot of total energy and entropy. Despite this, the extraordinary precision of the measurements is able to discriminate between these theories in the interaction energy, as given in Fig. 3. The NSR approach is seen to give the best fit to the experimental data below T_c (corresponding to $S_c\approx 2.3Nk_B$) and above $T=0.5T_F$ (corresponding to $S>3.5Nk_B$). This indicates that the simplest non-self-consistent T-matrix approximation captures the essential physics of strong pair fluctuations at both low (superfluid) and high (normal) temperatures. Around T_c, the experimental data shows evidence of what could be a first-order superfluid transition. However, due to "critical slowing-down," systematic experimental errors cannot be ruled out in this regime, if the magnetic field sweep is not quite adiabatic.

In the temperature region just above T_c, the NSR approach presumably does not fully capture the full effect of fluctuations, compared to the self-consistent $(GG)G$ theory above T_c. At the transition, from the experimental data one may determine experimentally a critical entropy $S_c/N\simeq 2.3k_B$ and a critical energy $E_c/N\simeq 0.86E_F$ in a trap. The critical temperature T_c/T_F in the case of a trap is difficult to determine, due to the unknown relation $S(T)$. The theoretical predictions are 0.29 [NSR], 0.21 [$(GG_0)G_0$ and $(GG)G$], and 0.27 [pseudogap model].

In a further comparison, we include in Fig. 3 a recent QMC calculation (thin solid line) of trapped Fermi gases [28]. There is a noticeable systematic difference between the QMC and experimental data at high entropy, but this is due to the improper use of an ideal gas approximation in the QMC estimates for large T. It is clear that the unitarity gas remains strongly interacting even close to the degenerate temperature (i.e., $S\simeq 5Nk_B$). Thus, a virial expansion of the equation of state up to the second order should be applied. Among all pair fluctuating theories, Fig. 3 shows that the pseudogap approximation gives poor agreement with thermodynamic data, though it is better than BCS mean-field theory—which completely ignores the pairing fluctuations. Therefore, the pseudogap model does not describe the strong fluctuations at unitarity as well as the full $(GG_0)G_0$ theory.

In conclusion, the accurate thermodynamic measurements at Duke University have allowed us to perform a test of strong-coupling *T*-matrix theories at unitarity. The simplest NSR approximation for the particle-particle *T* matrix is found to give the best quantitative description. Further work is needed to understand the reason for this, but we conjecture that it is related to scale-invariance symmetry in the unitarity limit. We conclude that for a strongly interacting Fermi gas near a Feshbach resonance, the NSR approximation is surprisingly useful.

We thank Allan Griffin and Edward Taylor for discussions and critical reading of the manuscript. We also thank V. K. Akkineni *et al.* for providing us with their QMC data. This research is supported by the Australian Research Council Center of Excellence program, NSF-China Grant No. 10774190, and NFRP-China Grants No. 2006CB921404 and No. 2006CB921306.

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