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Finite-temperature equation of state of polarized fermions at unitarity

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We study in a nonperturbative fashion the thermodynamics of a unitary Fermi gas over a wide range of temperatures and spin polarizations. To this end, we use the complex Langevin method, a first principles approach for strongly coupled systems. Specifically, we show results for the density equation of state, the magnetization, and the magnetic susceptibility. At zero polarization, our results agree well with state-of-the-art results for the density equation of state and with experimental data. At finite polarization and low fugacity, our results are in excellent agreement with the third-order virial expansion. In the fully quantum mechanical regime close to the balanced limit, the critical temperature for superfluidity appears to depend only weakly on the spin polarization.

Introduction – Without a doubt, one of the most intensely studied systems in recent years, at the interface of atomic, nuclear, and high-energy physics, is that of two-component fermions in the scale-invariant limit of infinite s -wave scattering length and effectively zero interaction range: the unitary Fermi gas (UFG) [1–4]. This system is now routinely realized to an excellent approximation with ultracold alkali atoms in several laboratories around the world (see Refs. [5–9] for reviews of theory and experiment) and simultaneously (though only approximately) in dilute neutron matter in neutron star crusts [10–12]. Because of the lack of scales characterizing the interaction between the fermions, all physical quantities at unitarity are fully determined by *universal* numbers in units of the fermion density [13] being the only scale of the system. This property renders the system relevant for such disparate energy scales as those of atomic and astro-physics, and has moreover been shown to reflect a nonrelativistic type of conformal invariance [14–17].

A peculiarity of the UFG is that it lies in the middle of the crossover between Bardeen-Cooper-Schrieffer (BCS) superfluidity and Bose-Einstein condensation (BEC), where the appearance of pseudo-gap phenomena and preformed Cooper pairs at high temperature appears possible [18–22]. This suggests intriguing connections to high- T_c superconductors. Due to such relevance of the UFG for various fields, the past two decades have seen uncounted studies exploring the properties of this crossover in the unpolarized limit both theoretically and experimentally [4]. Finite spin polarizations are even more challenging to tackle (see e.g. [23–27] for reviews, and [28–42] for experimental work) and therefore this case leaves us with many puzzles. At low temperatures, when the system is superfluid, a large enough polarization will destroy superfluidity [43, 44]. Precisely how that happens, and what other exotic superfluid phases may be traversed in the process, has remained a controversial topic not only for atomic superfluids but also for their quantum chromodynamics (QCD) counterparts, namely color super-

conductors [23]. Part of the challenge in answering such questions is that the UFG (not unlike QCD and many other systems) is a strongly correlated many-body system lacking a small parameter and therefore can only be tackled with nonperturbative methods. However, nonperturbative (semi-)analytic studies of such systems rely on some ansatz and conventional Monte Carlo (MC) calculations are unavailable at finite polarization due to the infamous sign problem.

In this work, we explore the *spin polarized* UFG at finite temperature, providing some of the essential measurable properties that characterize its universal thermodynamics, namely the density and magnetic equation of state (EOS). From those, differentiation yields static response functions such as the compressibility and magnetic susceptibility, while integration yields the pressure. To determine those EOSs, we implement a complex version of stochastic quantization known as the complex Langevin (CL) method [45], which we have developed and tested for spin- and mass-imbalanced one-dimensional nonrelativistic systems [46], including successful comparisons with exact answers in the ground state [47] and at finite temperature [48]. In the present work, we further validate our approach by comparing our results with the virial expansion and state-of-the-art MC calculations at zero polarization, eventually obtaining *ab initio* predictions for thermodynamic quantities of the UFG over wide temperature and polarization ranges.

Hamiltonian and method – Fermions in the unitary limit are governed by a Hamiltonian with a nonrelativistic dispersion relation and a zero-range interaction:

$$\hat{H} = \int d^3x \hat{\psi}_s^\dagger(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\psi}_s(\mathbf{x}) - g \int d^3x \hat{n}_\uparrow(\mathbf{x}) \hat{n}_\downarrow(\mathbf{x}),$$

where $\hat{\psi}_s^\dagger, \hat{\psi}_s$ are the fermion creation/annihilation operators for spin projection $s = \uparrow, \downarrow$ (summed over in the kinetic term), and the corresponding coordinate-space densities are $\hat{n}_s(\mathbf{x}) = \hat{\psi}_s^\dagger(\mathbf{x}) \hat{\psi}_s(\mathbf{x})$. Although we have written \hbar and the fermion mass m explicitly, we take

$\hbar = k_B = m = 1$ from this point on. The grand-canonical partition function then reads

$$\mathcal{Z} = \text{Tr} \exp \left[-\beta(\hat{H} - \mu_\uparrow \hat{N}_\uparrow - \mu_\downarrow \hat{N}_\downarrow) \right], \quad (1)$$

where μ_s is the chemical potential for spin $s = \uparrow, \downarrow$ particles, \hat{N}_s is the corresponding particle number operator, and $\beta^{-1} = T$ is the temperature. To tackle the strongly coupled many-body problem described by \mathcal{Z} , we put the system on a spacetime lattice (via a Suzuki-Trotter factorization) and introduce a path integral representation of the interaction by way of an auxiliary-field Hubbard-Stratonovich (HS) transformation. As those steps are rather standard (see e.g. [49]), we only state the result:

$$\mathcal{Z} = \int \mathcal{D}\sigma e^{-S[\sigma]}, \quad (2)$$

where $S[\sigma] = -\ln \det(M_\uparrow[\sigma]M_\downarrow[\sigma])$ is the action for the (real-valued) HS field σ and contains all the input parameters mentioned above. The details of the shape of the real-valued Fermi matrix $M_s[\sigma]$ can be found for instance in Ref. [49]. It is important to note here, however, that $M_\uparrow[\sigma]$ includes μ_\uparrow and not μ_\downarrow , and viceversa for $M_\downarrow[\sigma]$; i.e., we use an HS transformation that decouples the interaction in the density channel. As a result, in the unpolarized limit $\mu_\uparrow = \mu_\downarrow$, the fermion determinant is positive and the action is real, such that $e^{-S[\sigma]} \geq 0$ can be used as a probability measure in a Metropolis-based MC calculation, i.e. there is no sign problem in that case. On the other hand, for the polarized case $\mu_\uparrow \neq \mu_\downarrow$, such that $M_\uparrow[\sigma] \neq M_\downarrow[\sigma]$, and therefore S can be complex, which hinders the use of probabilistic MC approaches.

The aforementioned sign problem is well known and pervades MC approaches across all of physics [50], including high- T_c superconductors (due to strong repulsive interaction away from half filling) [51], nuclear structure (strong repulsive core, finite spin-isospin polarization) [52, 53], and QCD (at finite quark density) [54–57], to name a few. Recently, some progress has been made in understanding the sign problem as well as in its treatment with complex-plane methods such as the CL approach [45] and Lefschetz thimbles [58–62]. In essence, the CL algorithm implements an extension of conventional, Langevin-based stochastic quantization [63–65] to the case of complex-valued actions. As the Langevin equation uses S to evolve σ in its configuration space, a complex S naturally requires complexifying the HS field σ . Further details on the algorithm and our implementation can be found in Refs. [46, 48, 66–68]. Thus far, we have successfully applied such an approach to nonrelativistic fermions in 1D in a variety of situations, such as finite temperature and polarization [48], and mass asymmetry at zero temperature [47]. Those studies yielded an optimistic outlook for their higher-dimensional counterparts, i.e. this work. Still, a word of caution is in order

regarding this method. While conventional Metropolis-based methods are on solid mathematical footing at vanishing polarization, the CL approach remains a method under construction. A discussion of the issues is beyond the scope of this work, but these are being investigated by us and other groups in the lattice QCD area (see e.g. [69–73]). We emphasize that the calculations presented below display the same runtime features as our prior 1D studies which, together with the self-consistency of the results and the agreement with other methods in the balanced case and the virial expansion at finite polarization, gives some confidence on the reliability of the answers.

Results – To characterize the universal thermodynamics of the polarized UFG, we computed the density n , magnetization m , and normalized magnetic susceptibility $\bar{\chi}_M = \partial \bar{m} / \partial(\beta h)$ with $\bar{m} = m/n(\beta h=0)$ as functions of the dimensionless chemical potential $\beta\mu = \beta(\mu_\uparrow + \mu_\downarrow)/2$, and the dimensionless chemical potential difference $\beta h = \beta(\mu_\uparrow - \mu_\downarrow)/2$. The path integral form of the thermal expectation values of n and m is obtained by differentiating $\ln \mathcal{Z}$ with respect to μ and h . The magnetic susceptibility, which becomes the Pauli susceptibility in the noninteracting case, is then derived from the magnetic EOS. To evaluate such path integrals, we discretized spacetime into a (3+1)-dimensional lattice of spatial volume $V = L^3$, with $L = \ell N_x$, $N_x = 7, 9, 11$, lattice spacing $\ell = 1$, and periodic boundary conditions. For the temporal direction, we chose $N_\tau = 160$, with temporal lattice spacing $\tau = 0.05\ell^2$, and anti-periodic boundary conditions for the fermion fields. Note that, while we varied the spatial extent of the box in our calculations, we kept $\beta = \tau N_\tau = 8.0$ fixed. Our choice for the latter determines the thermal de Broglie wavelength $\lambda_T = \sqrt{2\pi\beta} \simeq 7.0$ being consistent with the continuum-limit window $1 = \ell \ll (\lambda_T, \lambda_F) \ll L = N_x \ell$, where $\lambda_F = 2\pi/k_F$ is the Fermi wavelength, and $k_F = (3\pi^2 n)^{-\frac{1}{3}}$ is the Fermi momentum at the given density. Thus, the computational challenge, besides the sign problem, is that of opening that window of scales by making N_x and β as large as possible, in that order, and staying in a dilute regime to suppress artifacts associated with the ultraviolet energy cutoff imposed by the lattice. Note that the reliability of calculations based on our present set of spacetime lattice parameters has been analyzed in detail in the past [74–79].

The bare coupling constant g in the Hamilton operator was fixed to the two-body bound-state threshold using Lüscher’s formula [80, 81], as in Ref. [82]. Under those conditions, we varied the asymmetry parameter over the range $\beta h \in [0.0, 2.0]$ (corresponding to $T \geq h/2$), and the chemical potential in the interval $\beta\mu \in [-3.0, 2.5]$, covering the semiclassical regime (at low fugacities $z_s = e^{\beta\mu_s}$, where the virial expansion is valid) to the fully quantum mechanical regime at large positive $\beta\mu$, including a small region below the superfluid transition temperature

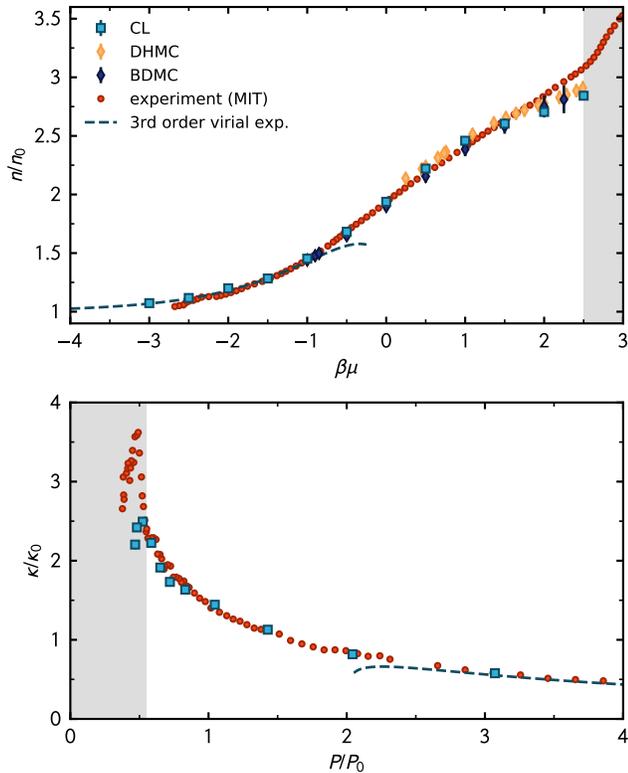


FIG. 1. Top: Density of the balanced UFG obtained by CL (blue squares), in units of the noninteracting unpolarized density n_0 as a function of the dimensionless average chemical potential $\beta\mu$. Also shown: third-order virial expansion (dashed line), experimental results of Refs. [83, 87] (red circles), and theoretical results obtained by bold diagrammatic Monte Carlo [87] (dark diamonds) and determinantal hybrid Monte Carlo [82] (light diamonds). Bottom: Compressibility κ as derived from the density EOS (see Supplemental Material) in units of its noninteracting ground-state value κ_0 , as a function of the pressure P normalized by the noninteracting ground-state pressure P_0 (blue squares), compared to experimental values [83] (red circles) and third-order virial expansion (dashed line). Statistical uncertainties for the CL results are on the order of the symbol sizes. Shaded areas indicate the superfluid phase.

for the unpolarized system, at $(\beta\mu)_c \simeq 2.5$ [83–86].

To validate our results, we use prior lattice MC [82], diagrammatic MC [87] and MIT experimental [83, 87] results obtained in the unpolarized limit (first measured in [88, 89] and computed with MC in [90]), as well as the third-order virial expansion at finite polarization, which reads

$$n - n_0 = \frac{Q_1}{V} \left[2\Delta b_2 z_\uparrow z_\downarrow + 3\frac{\Delta b_3}{2} (z_\uparrow^2 z_\downarrow + z_\uparrow z_\downarrow^2) \right], \quad (3)$$

$$m - m_0 = \frac{Q_1}{V} [\Delta b_3 (z_\uparrow^2 z_\downarrow - z_\uparrow z_\downarrow^2)], \quad (4)$$

where Q_1 is the two-species single-particle partition function, V is the spatial volume, and in the continuum $Q_1/V \rightarrow 2/\lambda_T^3$. The interacting total density is given by n , $n_0 = n_0(\beta\mu, \beta h)$ is the noninteracting total density, $m = n_\uparrow - n_\downarrow$ is the magnetization of the interacting system, and $m_0 = m_0(\beta\mu, \beta h)$ is the associated noninteracting magnetization. The above coefficients are $\Delta b_j = b_j - b_j^0$, where $b_j^0 = (-1)^{j-1} j^{-5/2}$ are the virial coefficients of the noninteracting gas, and $b_2 = 3/(4\sqrt{2})$, $b_3 \approx -0.29095$ (see, e.g., Refs. [36, 91]) are the coefficients of the unitary gas. The coefficient b_4 is also known for the unpolarized gas: $b_4 = 0.078(18)$ (see Ref. [92]), but two separate coefficients are needed at that order in the polarized case.

For the parameter region studied, we find that our $\beta h = 0$ results are in excellent agreement with the third-order virial expansion for $\beta\mu \lesssim -1$; see Fig. 1 for the density EOS and the isothermal compressibility $\kappa = (1/n)(\partial n/\partial P)|_T$ with P being the pressure and n being the total density. Moreover, our results reproduce closely the existing results from lattice MC [82], diagrammatic MC [87], and the MIT experiments [83, 87] in the unpolarized limit, up to $\beta\mu = 2.0$, which reflects the smallness of the systematic effects in that parameter range. The smoothness of the curve connecting the data points shows that statistical effects are also well controlled and are roughly of the size of the symbols. For $\beta\mu > 2.0$, on the other hand, systematic effects in all state-of-the-art calculations, namely finite-range and finite-volume effects, become more important and underlie the observed deviation from the MIT measurements at low temperature, i.e. close to and below the superfluid phase transition. Still, some indication of the appearance of the phase transition is visible in our present data as a sharp peak in the compressibility close to $P/P_0 \approx 0.5$, in accordance with experiment.

Given the excellent agreement of our results for the balanced UFG with existing theoretical and experimental data above the superfluid phase transition, we now proceed to the polarized case. In Fig. 2, we present our main results: density EOS normalized by the density of the noninteracting gas $n_0(\beta\mu, \beta h = 0)$ as a function of $\beta\mu$ (left panel) for $\beta h = 0, 0.4, \dots, 2.0$; magnetization (central panel) normalized by the interacting density of the *balanced* system $n(\beta\mu, \beta h = 0)$ as well as magnetic susceptibility (right panel) as a function of the asymmetry parameter βh for $\beta\mu = -3, -2, \dots, 2$.

For the density and magnetization EOSs, we again find excellent agreement with the virial expansion for sufficiently negative $\beta\mu$. However, we also observe that the regime of validity of the expansion appears to shrink as βh is increased, see left panel of Fig. 2. Indeed, for $\beta h = 2.0$, the third-order virial expansion clearly deviates from our nonperturbative results for $\beta\mu \gtrsim -1$, as opposed to the balanced case discussed above.

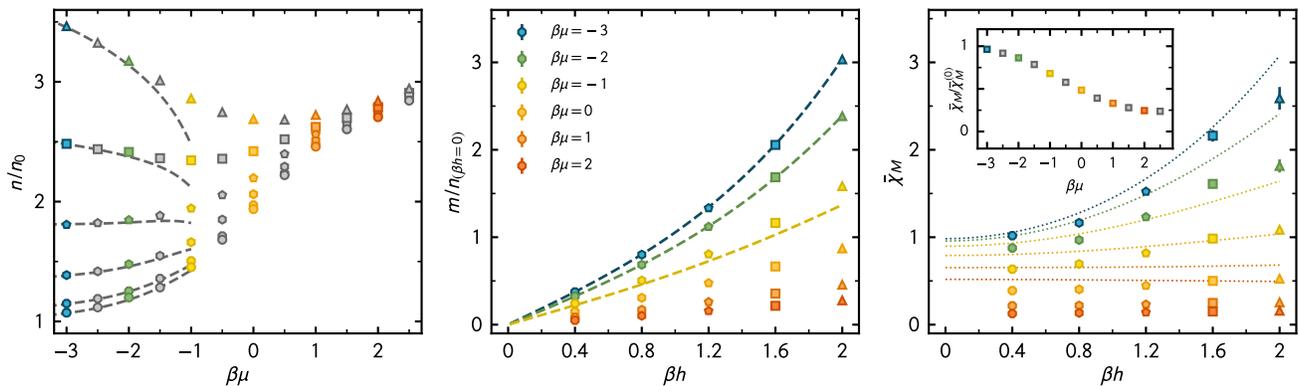


FIG. 2. Left: Density of the UFG in units of the noninteracting density from bottom to top: $\beta h = 0$ (circles), 0.4 (octagons), 0.8 (hexagons), 1.2 (pentagons), 1.6 (squares), 2.0 (triangles), compared to the third-order virial expansion (dashed lines). Colors encode fixed values of $\beta\mu$ shown in all panels. Center: Magnetization in units of the interacting density for the balanced system as a function of βh for several values of $\beta\mu$. For $\beta\mu \leq -1.0$, third-order virial expansion is shown with dashed lines. Right: Dimensionless magnetic susceptibility $\bar{\chi}_M$ as a function of βh (symbols) compared to the corresponding susceptibility of the free Fermi gas $\bar{\chi}_M^0$ (dotted lines) at equal chemical potential and asymmetry (color and shape coding as in other panels). Inset: Ratio $\bar{\chi}_M/\bar{\chi}_M^0$ as a function of $\beta\mu$ at $\beta h = 0.4$.

As $\beta\mu$ is increased, the EOSs obtained for different values of βh approach the EOS of the balanced system. This is not unexpected, as the relative asymmetry h/μ decreases when $\beta\mu$ is increased at fixed βh . Of course, the approach to the balanced EOS should happen at progressively larger values of $\beta\mu$ when βh is increased, which is indeed the case and can be seen in the left panel of Fig. 2. As the balanced system is known to be governed by a superfluid ground state above a critical value of $\beta\mu$, this observation also suggests that the critical temperature decreases with increasing spin asymmetry, in line with (semi-)analytic studies [25, 26, 84, 85, 93, 94] and lattice MC studies of a slightly spin-imbalanced UFG using reweighting techniques [95].

Our discussion of the density EOS at finite spin asymmetry carries over to the magnetization m (Fig. 2, center). Similar to the density, the results for m match the third-order virial expansion for large negative values of $\beta\mu$. As $\beta\mu$ is increased, however, our nonperturbative results clearly start to deviate from the virial expansion. For $\beta\mu = 2.0$, i.e. close to the critical value of the balanced system, we observe that m only shows a very mild dependence on βh . As m is expected to be small in the superfluid phase (the response to h being suppressed by the pairing gap, see e.g. [96]), our results suggest that the system remains close to the superfluid phase for $\beta h \lesssim 2$, provided that $\beta\mu$ is fixed close to its critical value $(\beta\mu)_c \simeq 2.5$ for the balanced case. Sufficiently below $(\beta\mu)_c$, i.e. at sufficiently high temperature, the system can easily “magnetize” by increasing βh .

To supplement our discussion of magnetic properties of the UFG, we also show results for the magnetic susceptibility $\bar{\chi}_M$, which measures the response under a variation of the spin asymmetry (Fig. 2, right panel). In the noninteracting gas at low effective magnetic field βh , the sus-

ceptibility is well approximated by the field-independent Pauli susceptibility. For negative $\beta\mu$, corresponding to the very dilute limit, our results for $\bar{\chi}_M$ of the UFG approach those for the free Fermi gas. Interestingly, even for $\beta\mu$ close the critical point, the functional form of the susceptibility of the interacting system is still very similar to that of the free Fermi gas, however, rescaled by a dimensionless factor. The latter is shown in the inset in the right panel of Fig. 2 at $\beta h = 0.4$.

Let us finally comment on the dependence of the superfluid critical temperature T_c on βh . As mentioned above, all of our results display a rather mild dependence on βh for $\beta\mu \gtrsim 2.0$, which suggests a rather mild dependence of T_c as well, at least in the range $0 \leq \beta h \sim 2.0$. This observation is also supported by a computation of the compressibility: as we increase βh , we only observe a very slight shift of the maximum to lower temperatures compared to the balanced case (see Supplemental Material). This shift appears to be smaller than in (semi-)analytic studies [25, 26, 84, 85, 93, 94]. However, further work is needed to resolve this dependence quantitatively.

Summary and conclusions – We carried out a nonperturbative characterization of the density and magnetization EOS of the UFG at finite temperature. To that end, we implemented a finite-temperature stochastic lattice approach that addresses the sign problem by going to the complex plane, i.e. we used the complex Langevin approach and presented our results as a function of $\beta\mu$ and βh . We emphasize that those results are experimentally testable predictions [97] for *universal* properties of quantum many-body physics in the unitary limit, as realized in particular with ultracold gases. In the unpolarized case, we recover state-of-the-art results. At finite polarization, our answers agree with the third-order expansion for $\beta\mu \lesssim -2.0$, where the expansion is expected

to be valid. As in our 1D studies [48], however, the expansion deteriorates as βh is increased. For increasing $\beta\mu$, we find that the density EOS at finite asymmetry approaches the EOS of the balanced system. That approach is “delayed” when βh is increased, suggesting a decrease of the critical temperature associated with the superfluid phase transition; this is as expected since h tends to facilitate Cooper pair breaking. Our results for the magnetization support this interpretation and suggest a mild βh dependence even up to $\beta h = 2.0$. The present work does not only set the stage for future *ab initio* studies of this dependence but also of key features in the low-temperature regime, such as phase separation associated with the Chandrasekhar-Clogston limit, which has already attracted tremendous attention for many years now, both from the experimental [28–30, 36, 37, 98] and theoretical side (see, e.g., Refs. [84, 99–105]).

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