Pressure, Compressibility, and Contact of the Two-Dimensional Attractive Fermi Gas

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Using *ab initio* lattice methods, we calculate the finite temperature thermodynamics of homogeneous two-dimensional spin-$1/2$ fermions with attractive short-range interactions. We present results for the density, pressure, compressibility, and quantum anomaly (i.e., Tan's contact) for a wide range of temperatures (mostly above the superfluid phase, including the pseudogap regime) and coupling strengths, focusing on the unpolarized case. Within our statistical and systematic uncertainties, our prediction for the density equation of state differs quantitatively from the prediction by Luttinger-Ward theory in the strongly coupled region of parameter space, but otherwise agrees well with it. We also compare our calculations with the second- and third-order virial expansion, with which they are in excellent agreement in the low-fugacity regime.

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Introduction.—Quantum mechanics in two spatial dimensions (2D) is a fascinating playground for understanding fundamental physics in a wide variety of situations. It represents a necessary (though often odd) crossover between the integrable systems that live in one spatial dimension (1D) and their much more challenging 3D counterparts. Interest in 2D ranges from basic theory and experiment to marketable technological applications. Among the most salient features and systems in 2D, we have the peculiar behavior of Berezinskii-Kosterlitz-Thouless (BKT) phase transitions [1], the possibility of understanding quark confinement analytically [2], anomalous scale invariance in nonrelativistic systems [3], the challenge of high-temperature superconductors [4], and, of course, graphene [5].

In recent years, experiments with ultracold atoms [6,7] have made clear progress towards a clean and systematic study of fermionic atom clouds in constrained or modulated optical traps, which closely resemble a 2D situation. These have been of singular interest due to their malleability: the interatomic interaction can be tuned essentially at will, low-temperature degenerate regimes can be reached, spin- and mass-asymmetric systems can be studied, and so on, as we briefly summarize next. Early observation of 2D systems was reported in Refs. [8,9]; radio frequency spectroscopy studies were carried out in Refs. [10,11]; the crossover from 2D to 3D was studied in Refs. [12,13] (see also Ref. [14]); the behavior of polarons was reported in Ref. [15]; the density distribution in a trap was shown in Ref. [16]; the viscosity was measured in Ref. [17]; and the contact was reported in Ref. [18]. More recently, the criterion for 2D dynamics was scrutinized in Ref. [19]; the pressure was measured in Ref. [20]; polarized systems were studied in Ref. [21]; and pair condensation and the BKT transition were observed in Refs. [22,23] (see also Ref. [24]).

As advances have thus been made towards understanding the thermodynamics, structure, and phases on the experimental side, theorists are once again faced with the challenge of strongly coupled regimes, which defy analytic approaches. Previous theoretical studies have characterized the crossover between Bose-Einstein condensation (BEC) and the Bardeen-Cooper-Schrieffer (BCS) pairing in 2D via mean-field analyses [25–27]. The first determination of the ground-state equation of state, however, appeared relatively recently in Ref. [28], which used the diffusion quantum Monte Carlo method. Even more recently, Ref. [29] performed an auxiliary-field quantum Monte Carlo study of the ground state where the pressure, contact, and condensate fraction were determined. At finite temperature, the equation of state (EOS) was first computed in the virial expansion in Ref. [30], and in the Luttinger-Ward approach in Ref. [31]. Pair correlations were investigated using the virial expansion at about the same time in Refs. [32,33] (the latter of which also analyzed Tan's contact). Collective modes were studied in Refs. [34–36], and the shear viscosity and spin diffusion in Ref. [37].

In this Letter, we offer a few essential pieces of the thermodynamic puzzle of attractively interacting fermions in 2D. We implement a lattice Monte Carlo (LMC) method to calculate the thermal and short-range correlation properties of the system along the 2D analogue of the BCS-BEC crossover. Specifically, we determine the density EOS, from which we extract the pressure and compressibility; all of these are experimentally measurable. To our knowledge, the present is the first fully nonperturbative, *ab initio* calculation of the EOS of this system at finite temperature, in particular covering the nonsuperfluid phase and pseudogap regime above the BKT transition. We also present here the first calculation of Tan's contact parameter [38–41] at finite temperature in 2D that is free of uncontrolled approximations.

Hamiltonian and many-body method.—The dynamics of dilute spin-$1/2$ nonrelativistic fermions with short-range interactions is governed by a Hamiltonian,

$$\hat{H} = \int d^2x \left[\sum_{s=\uparrow,\downarrow} \hat{\psi}_s^\dagger(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\psi}_s(\mathbf{x}) - g \hat{n}_\uparrow(\mathbf{x}) \hat{n}_\downarrow(\mathbf{x}) \right], \tag{1}$$

where $\hat{\psi}_s^\dagger, \hat{\psi}_s$ are the creation and annihilation operators in coordinate space for spin s particles, and $\hat{n}_s = \hat{\psi}_s^\dagger \hat{\psi}_s$ are the corresponding densities.

Recently [42], we performed a study similar to the one presented here, but in 1D. Here, we used the same methods (closely related to those that Refs. [43–45] used in 3D) but applied them in 2D. We placed the spin-$1/2$ fermions in a Euclidean spacetime lattice of extent $N_x^2 \times N_\tau$ with (anti-) periodic boundary conditions in space (time). A Trotter-Suzuki factorization followed by a Hubbard-Stratonovich transformation [46] allowed us to write the grand-canonical partition function as a path integral over an auxiliary field. That integral was evaluated using Metropolis-based LMC methods (see, e.g., Refs. [47,48]). We use units such that $\hbar = m = k_B = 1$, where m is the mass of the fermions. The physical spatial extent of the lattice is $L \times L$, where $L = N_x \ell$ and we take $\ell = 1$ to set the length and momentum scales. The extent of the temporal lattice is set by the inverse temperature $\beta = 1/T = \tau N_\tau$. The time step $\tau = 0.05$ (in lattice units) was chosen to balance temporal discretization effects with computational efficiency; in any case, those discretization effects are smaller than the statistical ones.

As in our previous study, the physical input parameters are the inverse temperature β, the chemical potential $\mu = \mu_\uparrow = \mu_\downarrow$, and the (bare, attractive) coupling $g > 0$, which determines the binding energy ϵ_B of the two-body problem (see below). We then form two dimensionless quantities: the fugacity $z = \exp(\beta\mu)$ and the dimensionless coupling strength $\beta\epsilon_B$. Using z and $\beta\epsilon_B$ as parameters facilitates comparisons with experiments, as well as with other theoretical approaches such as the Luttinger-Ward calculations mentioned above. For certain purposes below, we also use the scattering length a_{2D} as a scale, defined by $\epsilon_B = \hbar^2/(m a_{2D}^2)$, and also the Fermi energy $\epsilon_F = k_F^2/(2m)$, where $k_F = \sqrt{2\pi n}$ and n is the total density.

The 2D case we consider here, in contrast to its 1D and 3D analogues, is peculiar due to its anomalous scale invariance (see e.g. Ref. [49]). Indeed, the dimensions of $\hat{\psi}_s$ are of inverse length [in the natural units mentioned above; see Eq. (1)], such that g is dimensionless and therefore the system is classically (i.e., before accounting for quantum fluctuations) scale invariant. The appearance of a two-body bound state with binding energy ϵ_B for $g > 0$ is an example of a quantum anomaly: the classical scale invariance is broken by quantum effects. Notably, massless quantum chromodynamics in 3D, also a scale-free theory at the classical level, displays a similar feature. The anomaly in the present system is measured by the value of Tan's contact [3].

Our calculations are exact up to statistical and systematic uncertainties. To address the former, we took 1000 decorrelated samples for each data point in the plots shown below, which yields a statistical uncertainty on the order of 3%. The smoothness of our results show that those effects are indeed small. To address the systematic effects, one must approach the continuum limit. Two-dimensional problems are computationally inexpensive relative to full 3D problems, but they are still challenging. Therefore, in this first study we restricted ourselves to $N_x = 11, 15, 19$. The continuum limit is achieved by lowering the density while remaining in the thermodynamic regime. In turn, this is accomplished by increasing the lattice parameter β, ensuring that the thermal wavelength $\lambda_T = \sqrt{2\pi\beta}$ satisfies $\ell \ll \lambda_T \ll L$; at fixed z, this reduces the density. We used $\lambda_T \simeq 8.0$, which is well within said regime. We then studied whether our results collapse to a universal curve when β and g are varied while $\beta\epsilon_B$ is held fixed. Lattice sizes larger than $N_x = 19$ are computationally more expensive but not impractical; we chose to fix that size and cover a wider region of parameter space instead. Because our study proceeded at constant $\beta\epsilon_B$, increasing β implies reducing g, which results in smaller uncertainties associated with the temporal lattice spacing τ; these are expected to be on the order of 1% to 2% (see, e.g., Ref. [44]).

Analysis and results.—To characterize the thermodynamics of a strongly interacting system, as is our objective here, a simple yet extremely effective route is to first calculate the total particle number density $n = N/L^2$ (where $N = N_\uparrow + N_\downarrow$ and N_s is the particle number for spin $s = \uparrow, \downarrow$) as a function of the thermodynamic variables (temperature, chemical potential, and interaction strength, as mentioned above). The density has the added benefit over other quantities that its statistical-noise effects in a LMC calculation are relatively small. From n, one may determine the pressure P by performing a numerical integration along $\beta\mu$, and the compressibility κ by differentiation.

In Fig. 1 we show the density n as a function of the dimensionless parameters z and $\beta\epsilon_B$, defined above. The noninteracting result used as a scale in that figure is $n_0\lambda_T^2 = 4I_1(z)$, where $I_1(z) = z dI_0(z)/dz$, and

$$I_0(z) = \int_0^\infty dx\, x \ln(1 + z e^{-x^2}). \tag{2}$$

Our calculations, shown in Fig. 1, display a clear deviation from the Luttinger-Ward approach of Ref. [31] for $-2 \leq \beta\mu \leq 2$. This is not unexpected, as that regime is challenging for most many-body approaches: it is where quantum fluctuations are strongest (at a fixed $\beta\epsilon_B$). Away from that region, however, the agreement with Ref. [31] is satisfactory. Both calculations seem to heal together to the virial expansion result in the regime of large and negative $\beta\mu$. The starting point for this expansion is a Taylor expansion of the grand thermodynamic potential Ω in powers of z,

$$-\beta\Omega = Q_1(z + b_2 z^2 + b_3 z^3 + \cdots), \tag{3}$$

where $Q_1 = 2L^2/\lambda_T^2$ is the 2D single-particle partition function and b_n are the virial coefficients, which in general will be functions of the coupling strength $\beta\epsilon_B$. Thus, the virial expansion for the density reads

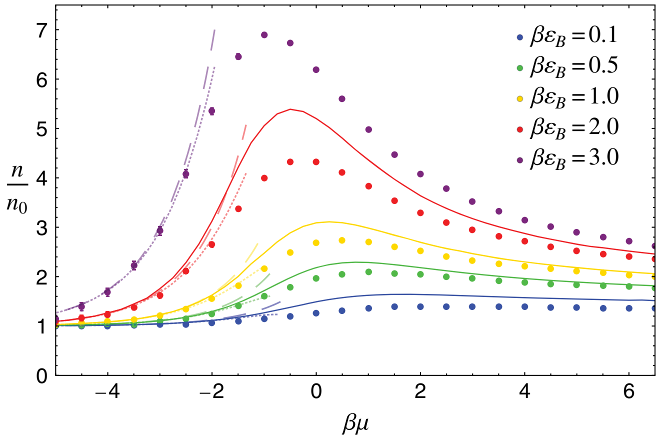

FIG. 1 (color online). Density equation of state, in units of the noninteracting density n_0 of spin-1/2 fermions in 2D, for coupling strengths $\beta\varepsilon_B = 0.1$, 0.5, 1, 2, 3 (from bottom to top), as a function of $\beta\mu$. The error bars reflect the statistical uncertainty. The solid colored lines show the Luttinger-Ward result of Ref. [31]. The long- and short-dashed lines show the second- and third-order virial expansion results, respectively.

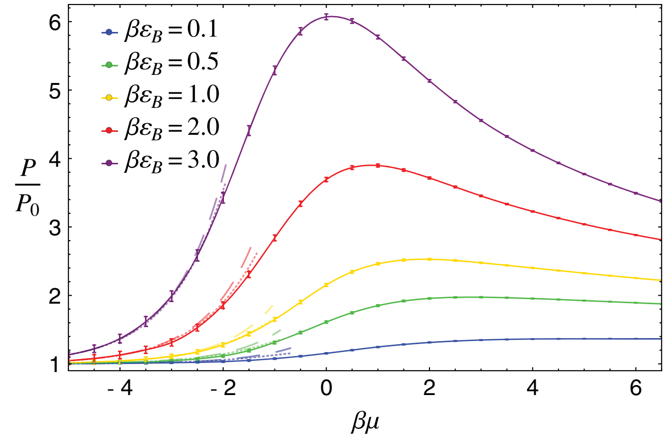

FIG. 2 (color online). Pressure, in units of the noninteracting pressure P_0, of spin-1/2 fermions in 2D for coupling strengths $\beta\varepsilon_B = 0.1, 0.5, 1, 2, 3$ (from bottom to top), as a function of $\beta\mu$. The error bars reflect the statistical uncertainty. The long-and short-dashed lines show the second- and third-order virial expansion results, respectively.

$n\lambda_T^2/2 = z + 2b_2z^2 + 3b_3z^3 + \cdots$, where the factor of 1/2 on the left-hand side comes from the number of fermion species. For the system studied here, the second-order coefficient b_2 is known analytically from the exact solution of the two-body problem (see, e.g., Refs. [32,34]):

$$b_2 = -\frac{1}{4} + e^{\beta\varepsilon_B} - \int_0^\infty \frac{dy}{y}\frac{2e^{-\beta\varepsilon_B y^2}}{\pi^2 + 4\ln^2 y}. \tag{4}$$

A calculation of b_3 can be found in Ref. [32].

To calculate the pressure P, we integrate as follows:

$$P\lambda_T^4 = 2\pi \int_{-\infty}^{\beta\mu} n\lambda_T^2 d(\beta\mu)', \tag{5}$$

where we have put everything in dimensionless form using the thermal wavelength scale. In Fig. 2 we show P, as obtained from the above formula, in units of the pressure of the noninteracting system $P_0\lambda_T^4 = 8\pi I_0(z)$. The virial expansion of Eq. (3) is used in this integration to complete the approach to the $z \to 0$ limit.

On the other hand, by taking a derivative of n, one obtains the isothermal compressibility,

$$\kappa = \frac{\beta}{n^2}\frac{\partial n}{\partial(\beta\mu)}\bigg|_\beta = \frac{\lambda_T^4}{2\pi}\frac{1}{(n\lambda_T^2)^2}\frac{\partial(n\lambda_T^2)}{\partial(\beta\mu)}\bigg|_\beta. \tag{6}$$

We report this quantity in Fig. 3, in units of its non-interacting counterpart κ_0, where (in dimensionless form) $\kappa_0\lambda_T^{-4} = (2/\pi)(n_0\lambda_T^2)^{-2}I_2(z)$, and $I_2(z) = zdI_1(z)/dz$.

To calculate the contact, we use the grand-canonical definition (see Refs. [32,39,41])

$$C \equiv \frac{2\pi}{\beta}\frac{\partial(\beta\Omega)}{\partial\ln(a_{2D}/\lambda_T)}\bigg|_{T,\mu}. \tag{7}$$

From here, it is easy to see that the virial expansion for C takes the form

$$\beta C = 2\pi Q_1(c_2z^2 + c_3z^3 + \cdots), \tag{8}$$

where $c_n = -\partial b_n/\partial\ln(a_{2D}/\lambda_T)$. Using Eq. (4), it is straightforward to obtain the exact continuum-limit answer:

$$c_2 = 2\beta\varepsilon_B e^{\beta\varepsilon_B}\left[1 + 2\int_0^\infty dy \frac{ye^{-\beta\varepsilon_B(y^2+1)}}{\pi^2 + 4\ln^2 y}\right]. \tag{9}$$

This result was likely used in Ref. [32], but we have not found the explicit formula itself anywhere.

In our LMC calculations, we determine the contact via the expectation value of the interaction energy $\hat{V}$. Using the definition of Eq. (7), along with $-\beta\Omega = \ln\mathcal{Z}$, where $\mathcal{Z}$ is the grand-canonical partition function, we obtain

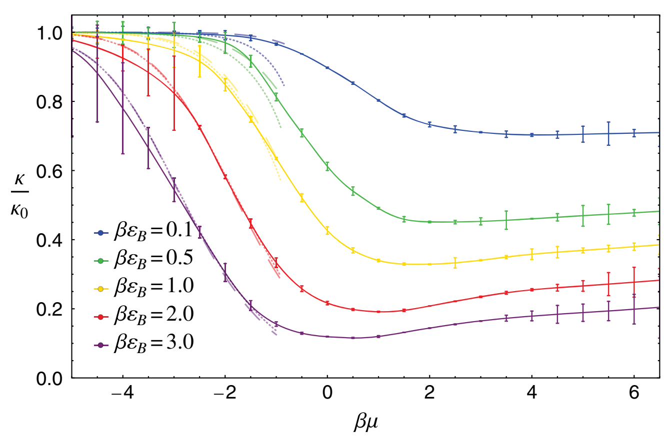

FIG. 3 (color online). Compressibility, in units of the non-interacting compressibility κ_0, of spin-1/2 fermions in 2D for coupling strengths $\beta\varepsilon_B = 0.1, 0.5, 1, 2, 3$ (from top to bottom), as a function of $\beta\mu$. The error bars reflect the difference between a smooth interpolation and the raw LMC data. The long- and short-dashed lines show the second-and third-order virial expansion results, respectively.

$$C = \frac{-2\pi}{\beta} \frac{\partial \ln \mathcal{Z}}{\partial \ln(a_{2D}/\lambda_T)} = -2\pi \langle \hat{V} \rangle \frac{\partial \ln g}{\partial \ln(a_{2D}/\lambda_T)}, \quad (10)$$

where we used the fact that $\hat{V}$ is a contact interaction, as in Eq. (1). The remaining factor on the right is given by the two-body problem. To turn this into an intensive, dimensionless quantity, we present results in the form $C/(Nk_F^2)$. In Fig. 4 we show our LMC results for this quantity as a function of T/T_F and the coupling strength $\beta\epsilon_B$, as well as selected lines of constant $\ln(k_F a_{2D})$. Corresponding to the latter, we have included ground-state quantum Monte Carlo (QMC) results [28] and experimental results at a finite temperature of $T/T_F = 0.27$ [18]. The experimental results largely agree with our calculations; however, the experimental errors and the maximum coupling calculated limit us from drawing any strong conclusions. On the other hand, we note that the contact is largely flat at constant $\ln(k_F a_{2D})$, which agrees qualitatively with the Luttinger-Ward approach of Ref. [31]. We regard all this as evidence that the ground-state QMC results (see also Supplemental Material [50]) are in very good agreement with our finite-T calculations, as the latter seem to approach the $T = 0$ results in that limit.

Our full set of contact calculations as a function of $\beta\mu$ can be found in the Supplemental Material [50]. We have also verified there the agreement with the continuum-limit second-order virial expansion result [using Eq. (9)] in the high-energy regime. Removing lattice effects in this regime is most demanding, which suggests that such systematic effects are well under control.

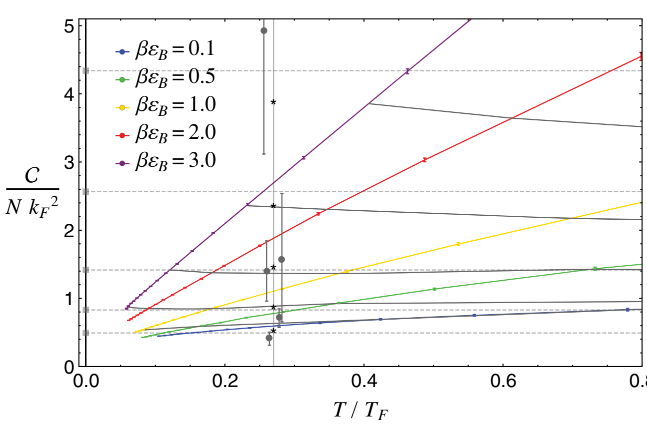

FIG. 4 (color online). Contact, in units of $1/(Nk_F^2)$, for spin-1/2 fermions in 2D for coupling strengths $\beta\epsilon_B = 0.1, 0.5, 1, 2, 3$ (from bottom to top), as a function of T/T_F. The error bars reflect the statistical uncertainty. Solid lines of gray across colored contact results indicate lines of constant $\ln(k_F a_{2D}) = 1.60, 1.21, 0.85, 0.53, 0.24$ from bottom to top. Corresponding experimental data at $T/T_F = 0.27$ from Ref. [18] given by solid circles (displaced about light gray line for visibility of error bars); corresponding Luttinger-Ward results at $T/T_F = 0.27$ from Ref. [31] are shown as black stars; and corresponding QMC calculations from Ref. [28] at $T/T_F = 0$ given by solid squares and dotted gray lines.

Summary and conclusions.—Using LMC methods, we have calculated the finite temperature thermodynamics of homogeneous two-dimensional spin-1/2 fermions with attractive short-range interactions. We have presented results for the density, pressure, compressibility, and Tan's contact for a wide range of temperatures (close to but above the superfluid critical temperature) and coupling strengths. Within our statistical and systematic uncertainties, our prediction for the density EOS differs from the prediction by Luttinger-Ward theory in a substantial region of parameter space. The general agreement is, nonetheless, exceptional. We have also compared our calculations of the density and pressure with the second- and third-order virial expansion, with which they agree remarkably well in the low-fugacity regime. Moreover, the agreement seems stronger with our results than with the Luttinger-Ward approach. Finally, we have presented a comparison of our calculation of the contact with previous ground-state calculations and finite temperature experimental data. A more complete representation of our data for the contact, including a comparison with the second-order virial expansion and an alternative temperature scale, appear in the Supplemental Material [50]. A further comparison of the pressure with experimental results is also shown there, as well as a consistency check with other calculations in the ground state.

Our results for the density and compressibility can also be compared with experiments. One of the motivations for the latter is that attractively interacting fermions in 2D are expected to undergo a BKT transition into a superfluid phase at low enough temperatures. We do not see, in the quantities studied here, any particular signature of the transition. However, we did not expect to see such a signal, either: to that end, it would be necessary to study the pair correlation function. We defer such calculations to future work.

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