Universality in one-dimensional fermions at finite temperature:
density, pressure, compressibility, and contact

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We present finite-temperature, lattice Monte Carlo calculations of the particle number density, compressibility, pressure and Tan’s contact of an unpolarized system of short-range, attractively interacting spin-1/2 fermions in one spatial dimension, i.e. the Gaudin-Yang model. In addition, we compute the second-order virial coefficients for the pressure and the contact, both of which are in excellent agreement with the lattice results in the low-fugacity regime. Our results, covering a wide range of couplings and temperatures, support the existence of a strong-coupling regime in which the thermodynamics of the system is markedly different from the non-interacting case; we compare and contrast our results with identical systems in higher dimensions.

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\textbf{Background.}— Universal aspects of strongly coupled non-relativistic many-body systems have been in the spotlight for the last decade. The realization and manipulation of these systems in the form of ultracold atomic clouds \cite{1}, followed by the enhanced understanding of universality in terms of underlying conformal invariance, equations of state, and the Tan relations \cite{2}, have clarified the central role of these simple systems for many-body quantum mechanics across all of physics.

Interest in the one-dimensional (1D) version of these systems has existed in the area of condensed matter for a long time (see e.g. \cite{3}), as many of these systems display quantum phase transitions, conformal invariance, and in some cases are exactly solvable (at zero temperature). Remarkably, 1D problems have also been studied in nuclear physics, where model calculations that resemble nuclear systems have often been performed (see e.g. \cite{4,5}), both for insight into the physics as well as to develop new many-body methods \cite{6}.

In spite of such broad interest, a precise characterization of attractively interacting fermions in 1D (e.g. in terms of the thermal equation of state and the contact) remains surprisingly absent from the literature. Such results are simultaneously a prediction for ultracold-atom experiments and a benchmark for many-body methods. In this work, we present such results, focusing on unpolarized spin-1/2 fermions with a contact interaction, i.e. the Gaudin-Yang model \cite{8}.

\begin{align}
\hat{H} = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 - \sum_{i<j} g \delta(x_i - x_j), \tag{1}
\end{align}

where the sums are over all particles. We cover weakly to strongly coupled regimes, as well as a wide range of temperatures, and show lattice Monte Carlo results for the particle number density $n$, pressure $P$, compressibility $\kappa$, and Tan’s contact $C$ \cite{9}. Furthermore, we use exact diagonalization on the lattice to obtain the second-order virial coefficient $b_2$ for the pressure and the leading-order coefficient $c_2$ for the contact. We also present analytic continuum results for $b_2$ and $c_2$.

\textbf{Methods and technical details.}— We employed a technique similar to that of Refs. \cite{10,12}, but applied in 1D. The two-species fermion system is placed in a Euclidean space-time lattice of extent $N_x \times N_z$, with periodic boundary conditions in the spatial direction, and anti-periodic in the time direction. A Trotter-Suzuki decomposition of the Boltzmann weight is implemented, followed by a Hubbard-Stratonovich transformation, allowing us to write the grand-canonical partition function in terms of a path integral over an auxiliary field. The path integral is evaluated using Metropolis-based Monte Carlo methods (see e.g. Ref. \cite{13}). Throughout this work, 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 $L = N_x \ell$, and we take $\ell = 1$ to set the length and momentum scales. The extent of the temporal lattice is set by the inverse temperature $\beta = 1/T = \tau N_z$.

The time step $\tau = 0.05$ was chosen to balance temporal discretization effects with computational efficiency; in any case, those discretization effects are smaller than our statistical effects.

The physical input parameters are the inverse temperature $\beta$, the chemical potential $\mu = \mu_\uparrow = \mu_\downarrow$, and the (attractive) coupling strength $g$. From these, we form two dimensionless quantities: the fugacity and the dimensionless coupling, given by

\begin{align}
z = \exp(\beta \mu) \quad \text{and} \quad \lambda^2 = \beta g^2, \tag{2}
\end{align}

respectively. In the grand-canonical ensemble, the density $n$ is an output variable, and therefore we use $\lambda$ instead of the $\gamma = g/n$ parameter often employed in 1D ground-state studies (see e.g. Refs. \cite{13,15}).

Note that, in 1D, fermions with a contact interaction are ultraviolet-finite, and as a consequence the bare coupling has a physical meaning. Indeed, in the continuum limit, $g = 2/a_0$, where $a_0$ is the scattering length for the symmetric channel (see e.g. Ref. \cite{16}). Using $z, \lambda$ as parameters will facilitate the comparison with experiments, as well as with other theoretical approaches.
Lattice calculations are exact, up to statistical and systematic uncertainties. To address the former, we have taken 5000 de-correlated samples for each data point in the plots shown below, which yields a statistical uncertainty of order 3–4%. To address the systematic effects, one must approach the continuum limit, which we discuss next. Because one-dimensional problems are computationally inexpensive, it is possible to calculate in large lattices, e.g. $N_x = 50–100$, and beyond, with modest computational resources. For such lattice sizes, the continuum limit is achieved by lowering the density, while still remaining in the many-particle, thermodynamic regime. Operationally, this is accomplished by increasing the lattice parameter $\beta$, ensuring that the thermal wavelength $\lambda_T = \sqrt{2 \pi \beta}$ satisfies $1/\ell \ll \lambda_T \ll L = \ell N_x$; at fixed $z$, this reduces the density. In our calculations, we have used $\lambda_T \simeq 3.5 \sim 7.0$ and $N_x = 81$, and thus checked that our results tend to the continuum limit. More specifically, this verification was performed by checking that our results collapse to the same (universal) curve when $\beta$ and $g$ are varied but $\beta g^2$ is held fixed. This “collapse” takes place at different rates for different parameter values, as we further explain below. Lattice sizes larger than $N_x = 81$ are computationally more expensive but certainly feasible; however, we chose to fix that size and cover a wider region of parameter space instead. Because our study proceeded at constant $\lambda^2 = \beta g^2$, increasing $\beta$ implies reducing $g$, which in turn results in smaller uncertainties associated with the temporal lattice spacing $\tau$ in the Trotter-Suzuki decomposition; these are expected to be of order $1–2\%$ (see e.g. Ref. [11]).

Results: General considerations.– We report our results in dimensionless form, by displaying quantities in units of their non-interacting counterparts at the same value of the input parameters, or by scaling them by the appropriate power of the thermal wavelength $\lambda_T = \sqrt{2 \pi \beta}$. Among our main results is the density equation of state $n(\lambda, \beta \mu)$, from which we obtain the pressure $P$ and the isothermal compressibility $\kappa$ by integrating and differentiating, respectively, with respect to the chemical potential. Our last Monte Carlo result is Tan’s contact $C$, which we determine by computing the average interaction energy. In addition to these quantities, we use exact diagonalization to compute the second-order virial coefficient for the pressure and density (i.e. $b_2$) and the corresponding (i.e. leading-order) coefficient for the contact (usually called $c_2$); for both of these we also provide analytic results.

Results: Density.– In Fig. 1 we show the density $n$ as a function of the dimensionless parameters $z, \lambda$, defined above. The non-interacting result is $n_0 \lambda_T = 2 \pi I_1(z)$, where $I_1(z) = z dI_0(z)/dz$, and $I_0(z) = \int_0^\infty dx \ln(1 + ze^{-x^2})$. The solid curve in Fig. 1 corresponds to a three-point moving average over an interpolation of the original Monte Carlo data. The error bars represent the difference between the original data and the moving average. For all $\lambda > 0$ there exists a strongly coupled regime around $\beta \mu = \ln z \simeq -1$, where the deviation from the non-interacting system is maximal. This effect is more pronounced for larger $\lambda$. By definition, the locus of the maxima (indicated in Fig. 1 with a dashed line) satisfies $n_0 \kappa_0 = n \kappa$, where $\kappa (\kappa_0)$ is the isothermal compressibility of the (non-interacting) system.

These results are, qualitatively, remarkably similar to those of Ref. [17]. In that work, the same equation of state was computed, for the same system, but in 2D. The similarity can be traced back to the fact that in both cases a bound state is formed as soon as interactions are turned on, i.e. the unitary limit coincides with the non-interacting limit. Therefore, increasing $\beta \mu$ along the line of constant physics (i.e. fixed $\lambda$) ultimately leads to a weak-coupling regime in 1D and 2D. In 3D, however, the analogous path drives the system deep into the non-trivial unitary limit. Indeed, Refs. [12] [18], for instance, do not see a peak in $n/n_0$, but rather a monotonically increasing function (see e.g. Fig. 4(a) in Ref. [18], or Fig. 4 in Ref. [12]).

To characterize the approach to the non-interacting limit in the region $\beta \mu > 0$, we performed fits to the density using the (purely phenomenological) functional form

$$n/n_0 = 1 + \alpha (\beta \mu)^{-\gamma},$$

where $\alpha, \gamma$ are functions of $\lambda$, as shown in Table I. For $\beta \mu \ll 0$, the virial expansion is applicable, for which

$$n \lambda_T/2 = z + 2b_2 z^2 + 3b_3 z^3 + \ldots,$$

and the factor of 1/2 on the left-hand side comes from the number of fermion species. In Table I we show the
virial coefficient \( b_2 \) obtained by exact diagonalization of the two-body problem on the lattice. The exact result for \( b_2 \) in the continuum limit, obtained by the same methods utilized in 3D (see e.g. Refs. [19, 20]), is

\[
b_2 = -\frac{1}{2\sqrt{2}} + \frac{e^{\lambda^2}}{\sqrt{2}} \text{erf}(\lambda/2),
\]

where \( \text{erf}(x) \) is the error function. From the above data, we determine other thermodynamic quantities, which furnish a prediction for ultracold atom experiments.

Table I. Fit parameters for the density equation of state, using the functional form \( n/n_0 = 1 + \alpha(\beta \mu)^\gamma \), second-order pressure virial coefficient \( b_2 \), and leading-order contact virial coefficient \( c_2 \), all as a function of the dimensionless coupling \( \lambda \).

For the non-interacting gas (\( \lambda = 0 \)), the virial coefficients are \( b_0 = (-1)^{n+1} n^{-3/2} \).

| \( \lambda \) | \( b_2(\text{lattice}) \) | \( c_2(\text{lattice}) \) | \( \alpha \) | \( \gamma \) |
|---|---|---|---|---|
| 0 | -0.35355 \ldots | 0 | 0.0 | - |
| 1.0 | 0.11(5) | 0.54(5) | 0.24(1) | 0.46(6) |
| 1.25 | 0.28(5) | 1.06(5) | 0.300(5) | 0.47(4) |
| 1.5 | 0.48(5) | 1.98(5) | 0.450(2) | 0.53(9) |
| 1.75 | 0.76(5) | 3.60(5) | 0.554(5) | 0.56(9) |
| 2.0 | 1.13(5) | 6.42(5) | 0.658(6) | 0.59(2) |
| 2.25 | 1.64(5) | 11.3(5) | 0.771(8) | 0.61(6) |
| 2.5 | 2.34(5) | 19.9(5) | 0.970(1) | 0.66(1) |
| 2.75 | 3.33(5) | 34.8(5) | 1.219(6) | 0.70(1) |
| 3.0 | 4.78(5) | 61.1(5) | 1.525(1) | 0.76(1) |

**Results: Pressure and compressibility.**– It is straightforward to obtain an estimate for the pressure by integrating \( n\lambda T \) over \( \log z = \beta \mu \). We take the \( z = 0 \) limit (i.e. \( \beta \mu \to -\infty \)) as a reference point. In practice, we verify that the data heals (within statistical uncertainties) to the virial expansion at low \( z \), and use that result (at second order) to complete the integration to \( z = 0 \). In that limit the pressure vanishes, such that

\[
\frac{P\lambda^3}{\theta} = 2\pi \int_{-\infty}^{\beta \mu} n\lambda T \, d(\beta \mu). \tag{6}
\]

The results for \( P \), in units of the non-interacting pressure \( P_0 \), are shown in Fig. 2. Note that \( P_0\lambda^3 = \sqrt{16\pi} I_0(z) \), where \( I_0(z) \) is given above. By taking a derivative of \( n \) one obtains the isothermal compressibility,

\[
\kappa = \frac{\beta}{n^2} \frac{\partial n}{\partial (\beta \mu)} = \frac{\lambda^3}{2\sqrt{2\pi}} \frac{\partial (n\lambda T)}{\partial (\beta \mu)} \bigg|_{\beta} \bigg|_{\beta}. \tag{7}
\]

We report this quantity in Fig. 3 in units of its non-interacting counterpart \( \kappa_0 \), where (in dimensionless form)

\[
\kappa_0\lambda^3 = \pi^{-3/2}(n_0\lambda_T)^{-2} I_2(z), \quad \text{and} \quad I_2(z) = z dI_1(z)/dz.
\]

As expected, in the limits of large \( \beta \mu \) (both positive and negative) \( \kappa \) tends to \( \kappa_0 \). On the other hand, in the strongly interacting region \( \kappa \ll \kappa_0 \), i.e. the system is less compressible than in the non-interacting regime.

We attribute this to the formation of localized di-fermion molecules and Pauli exclusion.

**Results: Contact.**– Knowing the density as detailed above, one may use the Maxwell relation between \( n \) and \( C \) (see Refs. [11, 21, 22]), which in dimensionless form reads

\[
\frac{z}{\theta} \frac{\partial (\beta^2 C)}{\partial z} \bigg|_{\lambda, T} = \frac{\lambda^2}{2\sqrt{2\pi}} \frac{\partial (n\lambda T)}{\partial \lambda} \bigg|_{z, T}. \tag{8}
\]

Alternatively, one may use the interaction energy \( \langle \hat{V} \rangle \). Starting from the definition in 1D,

\[
\frac{C}{\beta \lambda T} \frac{\partial (\beta \Omega)}{\partial (a_0/\lambda T)} \bigg|_{\mu, T}, \tag{9}
\]

where \( \Omega \) is the grand thermodynamic potential, the contact can be shown, using the Feynman-Hellman theorem,
to be given by

$$C = -g(\hat{V}).$$

(10)

Note that $C$ can be made dimensionless and intensive by multiplying it by $\lambda_T^2/L$. On the other hand, the virial expansion for $Q$ reads $-\beta Q = Q_1 (z + b_2 z^2 + b_3 z^3 + \ldots)$, where $Q_1 = 2L/\lambda_T$ is the single-particle partition function, and the virial coefficients $b_n$ are the same as those for the density appearing in Eq. 4. Thus, the virial expansion for $C$ takes the form

$$\beta C = \frac{2}{\lambda_T} Q_1 (c_2 z^2 + c_3 z^3 + \ldots),$$

(11)

where

$$c_n = -\frac{\partial}{\partial (a_0/\lambda_T)} \sqrt{\frac{2}{\pi}} \frac{\partial n}{\partial \lambda}.$$  

(12)

Our definition for the $c_n$ coefficients coincides with that of Ref. [23]. From our calculation of the virial coefficient $b_2$, we obtain $\partial b_2/\partial \lambda$; the resulting $c_2$ is shown in Table I. The exact continuum result (based on Eqs. 5 and 12) is

$$c_2 = \frac{\lambda^2}{\pi} - \frac{\lambda^3}{4\sqrt{\pi}} \frac{2}{\exp(\lambda/2)}.$$  

(13)

In Fig. 4 we show our results for the contact, including the leading-order virial expansion (inset). We show statistical error bars in the inset; in the main plot, the smoothness of the results across $\beta \mu$ indicate that the statistical effects are of the order of the size of the symbols. As seen in the inset, the data captures the correct asymptotic behavior at small $z$ for all $\lambda$, but the agreement slowly deteriorates at large $\lambda$, suggesting that the virial expansion breaks down earlier in that regime. For $\beta \mu > 1$ the contact satisfies

$$C^{\beta^2/(2Lx^2)} = \langle \hat{n}_1 \hat{n}_2 \rangle / \beta \rightarrow \zeta_1 \beta \mu + \zeta_2,$$  

(14)

where we find $\zeta_1 = 0.35(1)$ is nearly $\lambda$-independent and therefore entirely universal; it is in fact a feature of density-density correlations in the non-interacting gas that leaves an imprint at all couplings. On the other hand, as is evident from the plot, $\zeta_2$ is approximately linear in $\lambda$ at large $\beta \mu$: $\zeta_2 \approx a + b \lambda$, and we find $a = 3.09(1)$ (at $\beta \mu = 10$) and $b = 0.348(3)$. Analytic estimates in the absence of interactions yield $\zeta_1 = 1/\pi = 0.318\ldots$ and $a = \beta \mu/\pi$. Although much is known about $C$ in various situations (see e.g. Ref. [24] for a review), the temperature dependence in 1D shown here does not appear anywhere else in the literature, to the best of our knowledge.

Summary and Conclusions.– We have performed a fully non-perturbative, controlled study of the thermodynamics of the Gaudin-Yang model (i.e., a one-dimensional, two-species Fermi system, with short-range, attractive interactions). We employed lattice Monte Carlo methods that have been successfully utilized before for similar studies, and discussed statistical and systematic uncertainties. We report here on several quantities, namely the density, pressure, contact and leading virial coefficients, in all cases covering weakly to strongly coupled regimes (as characterized by values of the dimensionless parameter $0 \leq \beta^2 \leq 16.0$), as well as low to high temperatures (as characterized by $-5.0 \leq \beta \mu \leq 8.0$, which ranges from the semi-classical regime $\beta \mu < -1.0$ to the deep quantum regime $\beta \mu > 1.0$). Our results for the density equation of state display a behavior similar to that observed in 2D systems: A regime exists around $\beta \mu = \ln z \sim -1$ in which deviations from the non-interacting case are maximal. As $z$ is increased from $z \ll 1$ (the semi-classical regime where the virial expansion is valid) this strongly coupled regime is (roughly) accompanied by the onset of quantum fluctuations at $\beta \mu = \ln z \sim 0$.

Although certain 1D Fermi systems are exactly solvable via the Bethe ansatz [25], the latter is restricted to uniform systems in the ground state (or close to it [27]). Indeed, finite temperature studies require the thermodynamic Bethe ansatz, which involves solving an infinite tower of coupled non-linear integral equations [27]. Regardless, it is somewhat surprising that a thorough numerical characterization of this simple system, as a benchmark for many-body methods, is absent from the literature, to the best of our knowledge. To remedy this situation, we have characterized the universal thermodynamics of this system as much as possible.

Finally, our results constitute predictions for experiments with ultracold atoms in highly elongated optical traps. These are now realized using modulated potentials. Furthermore, this study is readily generalizable to...
a higher number of fermion species, which are expected to be experimentally available in the near future [28].

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