Determination of Scale-Invariant Equations of State without Fitting Parameters: Application to the Two-Dimensional Bose Gas Across the Berezinskii-Kosterlitz-Thouless Transition

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We present a general "fit-free" method for measuring the equation of state (EoS) of a scale-invariant gas. This method, which is inspired from the procedure introduced by Ku *et al.* [Science 335, 563 (2012)] for the unitary three-dimensional Fermi gas, provides a general formalism which can be readily applied to any quantum gas in a known trapping potential, in the frame of the local density approximation. We implement this method on a weakly interacting two-dimensional Bose gas across the Berezinskii-Kosterlitz-Thouless transition and determine its EoS with unprecedented accuracy in the critical region. Our measurements provide an important experimental benchmark for classical-field approaches which are believed to accurately describe quantum systems in the weakly interacting but nonperturbative regime.

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Homogeneous matter at thermal equilibrium is described by an equation of state (EoS), i.e., a functional relation between thermodynamic variables of the system. While the EoS is analytically known for ideal gases, one must resort to approximations or numerical calculations to determine the EoS of interacting fluids, which must then be compared to experiments. Thanks to a precise control of temperature, confining potential, and interaction strength, cold atomic gases constitute a system of choice for the experimental determination of quantum matter EoS [1]. While performed on atomic systems, such measurements often provide crucial insight on generic physical problems, well beyond the atomic physics perspective. Prominent examples are the recent measurements of the EoS of atomic Fermi gases [2–5], which provided a precious quantitative support for our understanding of strongly interacting fermions at low temperatures. Another important paradigm accessible to atomic gases is found in two-dimensional quantum systems, where the low temperature state is established via a defect-driven transition. This generic phenomenon of two-dimensional systems is described by the celebrated Berezinskii-Kosterlitz-Thouless (BKT) theory, with a scope that ranges from superconductivity to quantum Hall bilayer physics to high energy physics.

In this context, the weakly interacting two-dimensional Bose gas is of particular interest as it supports the fundamental principles of the BKT theory, while allowing for a simplified theoretical description. Indeed, for small enough interparticle interactions, the thermodynamics of the two-dimensional Bose gas is well captured by a classical-field model [6,7], which is itself described by a dimensionless coupling constant and exhibits scale invariance [8]. In general, scale invariance occurs in any fluid where no explicit energy or length scale is associated with the (binary) interaction potential. For the weakly interacting two-dimensional case, the 3D scattering length is normalized by the extension of the system in the third dimension, and this dimensionless ratio characterizes the effective 2D interaction strength. Scale invariance also occurs in the unitary Fermi gas, where the scattering length describing s-wave interactions diverges (for a review, see [12]). This property considerably simplifies the EoS structure, as general dimensionless quantities such as the phase space density $\mathcal{D}$ which usually depend separately on the chemical potential μ and the temperature T can only be expressed as the ratio $\mu/k_{\mathrm{B}}T$ owing to the absence of other energy scales [13,14].

The usual method for determining the EoS of a cold atomic gas starts with the measurement of the density distribution $n(\boldsymbol{r})$ in a smoothly varying, confining potential $V(\boldsymbol{r})$. Using the local density approximation (LDA), the measured $\mathcal{D}(\boldsymbol{r})$ is linked to that of a uniform fluid with the same interaction strength and temperature, and with chemical potential $\mu(\boldsymbol{r}) = \mu - V(\boldsymbol{r})$, μ being its value at the center of the trap [1]. For a given realization of the gas, T and μ are obtained by comparing the low-density wings of $n(\boldsymbol{r})$ with the known theoretical result for a dilute fluid. However, any systematic error in the determination of the density, e.g., due to imperfect calibration of the probing system, will lead to inaccurate values of μ and T and thus

affect the measurement of the EoS $\mathcal{D}(\mu, T)$. Recently, an alternative fit-free method that does not suffer from this limitation has been put forward in [4] for the measurement of the EoS of the scale-invariant 3D Fermi gas. It is based on the use of two specific thermodynamic variables, pressure and compressibility; in addition, absolute energy scales T and μ were replaced by a single relative scale $d\mu$, which was itself determined by the LDA through $d\mu = -dV$.

The purpose of the present Letter is twofold. First, we describe a method that generalizes the procedure introduced in [4], which does not rely on specific thermodynamic variables but rather provides a generic formalism that can readily be applied to other quantum systems. Second, we implement this method on a two-dimensional (Bose) fluid, for which the spatial density $n(\boldsymbol{r})$ is directly accessible from an image of the cloud. The precision of the reconstructed EoS makes it suitable for a quantitative comparison to the classical-field Monte Carlo calculation [7] in the critical region, which could not be conclusive from previous measurements [13,14]. Our measurement, with a relative statistical error smaller than 1% on the detectivity, is in excellent agreement (better than 5%) with the prediction obtained from [7] at the critical point and deeper in the superfluid regime. In the normal regime close to the transition point, we observe a deviation on the order of 15%, which might be due to beyond classical-field effects.

We start our analysis by considering an atomic gas in thermodynamic equilibrium confined in a known potential $V(\boldsymbol{r})$. The only hypothesis for the method is the LDA, which entails that $n(\boldsymbol{r})$ depends on position only through the local value of the trapping potential: $n(\boldsymbol{r}) = n[V(\boldsymbol{r})]$. Although this method is applicable to any dimension, we focus here on the particular case of the two-dimensional gas for the sake of clarity. Let us introduce the energy $E[V(\boldsymbol{r}))]$ with $\boldsymbol{r} = (x, y)$, defined by [15]

$$E = \frac{\hbar^2}{m} n, \tag{1}$$

which we want to combine with other relevant energies in order to form useful dimensionless variables. Though no absolute energy scales are readily available, a relative energy scale is provided by the variation of the trapping potential $\mathrm{d}V$. Furthermore, quantities formed in this manner are directly connected by the LDA to the properties of the uniform gas using the relation $d\mu = -dV$. Thus, we define the dimensionless quantities

$$X_\nu \equiv E^{\nu-1} \frac{\partial^\nu E}{\partial \mu^\nu} = (-1)^\nu E^{\nu-1} \frac{\mathrm{d}^\nu E}{\mathrm{d}V^\nu}, \tag{2}$$

where ν is an integer. By convention, $X_0 = 1$ and a negative ν will instead correspond to $|\nu|$ successive integrations of E with respect to V, with, for example,

$$X_{-1} = \frac{1}{E^2} \int_V^\infty E(V') dV'. \tag{3}$$

From a given image of the gas $n(\boldsymbol{r})$, one can thus construct all functions $X_\nu(V)$. In the case of a scale-invariant system, the knowledge of a single thermodynamic variable X_ν is sufficient to determine the state of the fluid and, hence, the values of all other variables $X_{\nu'}$. In other words, all individual measurements must collapse on a single line in each plane $\{X_\nu, X_{\nu'}\}$, irrespective of their temperature and chemical potential. Such a line is a valid EoS of the fluid under consideration.

Once the X_ν are known, all other thermodynamic quantities can be determined, up to an integration constant. In particular, one can derive the phase-space density $\mathcal{D}$ and the ratio $\alpha = \mu/k_\mathrm{B}T$. Let us suppose that a point $(X_\nu^{(0)}, X_{\nu'}^{(0)})$ can be identified in a known portion of the EoS and that it corresponds to the values α_0 and $\mathcal{D}_0$. The link between the set $\{X_\nu\}$ and $(\alpha, \mathcal{D})$ is provided by

$$\mathcal{D}(X_\nu^{(1)}) = \mathcal{D}_0 \exp\left(\int_{X_\nu^{(0)}}^{X_\nu^{(1)}} \frac{X_1}{(\nu-1)X_1X_\nu + X_{\nu+1}} dX_\nu \right), \tag{4}$$

$$\alpha(X_\nu^{(1)}) = \alpha_0 + \frac{1}{2\pi} \int_{X_\nu^{(0)}}^{X_\nu^{(1)}} \frac{\mathcal{D}(X_\nu)}{(\nu-1)X_1X_\nu + X_{\nu+1}} dX_\nu. \tag{5}$$

The determination of $(\alpha, \mathcal{D})$ thus requires the knowledge of a triplet $\{X_1, X_\nu, X_{\nu+1}\}$. This requirement can be weakened by choosing $\nu = 1$ or $\nu = -1$, in which case only the pairs $\{X_1, X_{-1}\}$ or $\{X_1, X_2\}$ are needed.

We illustrate this general procedure with a few examples. For the simple case of a Maxwell-Boltzmann gas, the EoS in terms of the X_ν's can be obtained analytically, and one gets, for example, $X_1X_{-1} = 1$ and $X_2 = X_1^2$. For an interacting 2D gas, the EoS is not known analytically; however, for the bosonic case, it can be approximated in two limiting cases. For $\mu < 0$, the gas is only weakly degenerate and the mean-field energy of an atom in the gas can be written as $2\tilde{g}(\hbar^2 n/m)$, where the dimensionless coefficient $\tilde{g}$ (assumed here to be $\ll 1$) characterizes the strength of the interaction. The thermodynamics is then well described by the prediction of the Hartree-Fock theory [16],

$$\mathcal{D} = -\ln(1 - e^{\alpha - \tilde{g}\mathcal{D}/\pi}), \tag{6}$$

from which we extracted numerically the values of X_{-1} and X_1 and plotted the corresponding EoS in Fig. 1. In the opposite case of a strongly degenerate gas (with a chemical potential that is positive and larger than $k_\mathrm{B}T$), the gas is described by the Thomas-Fermi equation $\mathcal{D} = 2\pi\alpha/\tilde{g}$. All X_ν are then constant, with $X_{-1} = \tilde{g}/2$, $X_1 = 1/\tilde{g}$, and $X_2 = 0$.

We now turn to the practical implementation of this method for processing data obtained with a quasi-2D

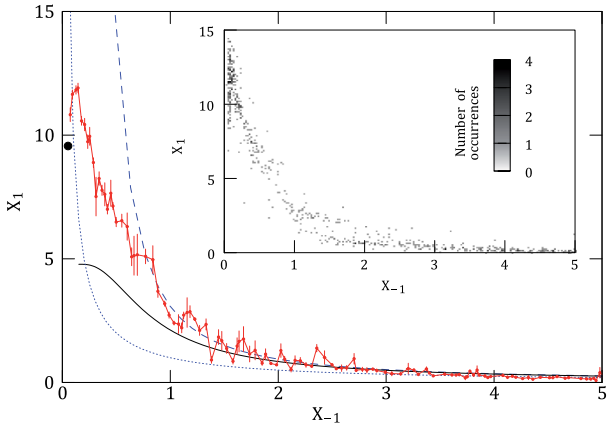

FIG. 1 (color online). Determination of the EoS with variables X_{-1} and X_1, along with known limits. The simple cases of the ideal Bose gas (Boltzmann gas) are shown as a blue dashed (dotted) line. The known limits of the EoS of the weakly interacting 2D Bose gas are indicated by a black point for the Thomas-Fermi limit and by a black solid line for the Hartree-Fock mean-field theory. The red line results from the averaging over all the separate intensity profiles, with the error bars corresponding to the standard error introduced by the averaging procedure. The data shown here contain ~100 different values of X_{-1}. Inset: Distribution of measured values of X_{-1} and X_1. The gray level indicates the number of individual data points falling in each pixel.

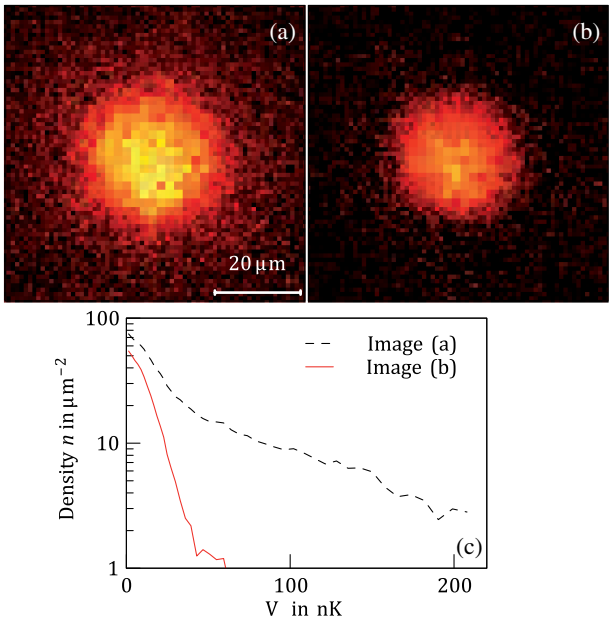

FIG. 2 (color online). (a) and (b): Density distributions of 2D atomic samples of ^{87}Rb corresponding to a partially degenerate (a) and a strongly degenerate cloud (b). (c): Corresponding function $n[V(\boldsymbol{r})]$ resulting from azimuthal averaging. The distributions are obtained with high intensity imaging.

rubidium gas. Our experimental preparation follows along the lines detailed in [14,17]. We start with a 3D gas of ^{87}Rb atoms, confined in their $F = m_F = 2$ state in a magnetic trap. To create a 2D system, we shine an off-resonant blue-detuned laser beam on the atoms, with an intensity node in the plane $z = 0$. The resulting potential provides a strong confinement perpendicular to this plane, with oscillation frequency $\omega_z/2\pi = 1.9(2)$ kHz, which decreases at most by 5% over typical distribution radii. This corresponds to the interaction strength $\tilde{g} = \sqrt{8\pi}a/l_z \approx 0.1$, where a is the 3D scattering length and $l_z = \sqrt{\hbar/m\omega_z}$ [18]. The energy $\hbar\omega_z$ is comparable to the thermal energy $k_B T$, which ensures that most of the atoms occupy the ground state of the potential along z (see [14] and [19]). The magnetic trap provides a harmonic confinement in the xy plane, with mean oscillation frequency $\omega_r/2\pi = 20.6(1)$ Hz. *In situ* density distributions of our clouds are measured via absorption imaging with a probe beam perpendicular to the atomic plane. For the analysis presented below, we used a data set of 80 samples, with temperatures ranging from 30 nK to 150 nK and atom numbers from 25 000 to 120 000.

In Fig. 2 we show typical density distributions of 2D atomic clouds, together with the corresponding function $n[V(\boldsymbol{r})]$. The cloud (a) exhibits a significant thermal fraction, contrarily to cloud (b), which is essentially in the Thomas-Fermi regime. The latter illustrates the power of this fit-free method since it can be incorporated as such in our determination of the EoS. On the other hand, it would be discarded in a conventional approach, owing to the impossibility of assigning it a temperature.

Though both choices of variables (X_{-1}, X_1) and (X_1, X_2) are, in principle, possible, the latter requires the experimental evaluation of a second-order derivative, which often suffers from a poor signal-to-noise ratio. By contrast, the choice (X_{-1}, X_1), also adopted in [4] when writing the EoS in terms of pressure and compressibility, appears particularly robust [23]. For each image, we perform an azimuthal average and compute a set of ≈70 data points (X_{-1}, X_1), where the low (high) values of X_{-1} correspond to the high (low) density regions of the image.

In a first step, we combine all sets obtained from images acquired at various temperatures and various atom numbers to test the scale invariance. As explained above, each individual measurement should sit on the same universal curve in the (X_{-1}, X_1) plane, provided the interaction strength $\tilde{g}$ is constant. We show in the inset of Fig. 1 the repartition of data points in the (X_{-1}, X_1) plane, which fall as expected around a single curve. In the main panel we plot the corresponding average curve, which provides the EoS of our gas [24]. In order to reexpress this EoS in terms of the more traditional variables α and $\mathcal{D}$, we now need to apply the transformations of Eqs. (4) and (5). However, these transformations must be adapted to account for possible imperfections in the calibration of the detectivity of our imaging setup. Indeed, as in most cold atom experiments, we only measure the density up to a global

multiplicative factor β [25], which is defined as the ratio between the unknown actual absorption cross-section and the ideal one expected for monochromatic probe light in the absence of stray magnetic fields. Taking this calibration factor into account amounts to replacing Eqs. (4) and (5) by

$$\mathcal{D}(X_\nu^{(1)}) = \mathcal{D}_0 \exp\left(\int_{X_\nu^{(0)}/\beta^\nu}^{X_\nu^{(1)}/\beta^\nu} \frac{X_1}{(\nu-1)X_1X_\nu + X_{\nu+1}} dX_\nu\right), \quad (7)$$

$$\alpha(X_\nu^{(1)}) = \alpha_0 + \frac{\beta}{2\pi}\int_{X_\nu^{(0)}/\beta^\nu}^{X_\nu^{(1)}/\beta^\nu} \frac{\mathcal{D}(X_\nu)}{(\nu-1)X_1X_\nu + X_{\nu+1}} dX_\nu, \quad (8)$$

where the bounds of the integrals now depend on β and where $X_\nu^{(0)}/\beta^\nu$ corresponds to the reference values α_0 and $\mathcal{D}_0$. The value of β is *a priori* unknown; however, it can be determined by fitting the measured EoS to the Hartree-Fock mean-field theory, which is a good approximation in the region $\alpha < 0$. This procedure applies to any other quantum gas, provided one has a good knowledge of the EoS in a given segment of the parameter space.

We choose the bound of Eqs. (7) and (8) at $X_{-1}^0 = 3$, which corresponds to a phase-space density $\mathcal{D}_0 = 1.45$ and $\alpha_0 = -0.22$, well within the Hartree-Fock mean-field regime, and find a detectivity factor $\beta = 0.456(1)$ [26]. The EoS in terms of the variables $(\alpha, \mathcal{D})$—obtained after a small correction due to excited states of the z motion (see [19])—is shown in Fig. 3(a), along with the numerical prediction $\mathcal{D}_{\rm th}$ [7]. The reconstructed EoS is remarkably smooth and does not display any particular feature at the transition point. This observation is also made on the EoS for pressure, entropy, and heat capacity [19]. This illustrates the "infinite-order" nature of the BKT transition, which is not associated with any singularity of thermodynamic quantities [27], as opposed to phase transitions driven by the breaking of a continuous symmetry, such as the second-order lambda transition observed at MIT [4]. To compare quantitatively the reconstructed EoS with the numerical prediction, we plot the quantity $\mathcal{D}/\mathcal{D}_{\rm th} - 1$ in Fig. 3(c) and find that it lies consistently below 15%, and even below 5% around the phase transition, which occurs at $\mu_C/k_{\rm B}T \approx 0.17$ [7]. The deviation observed in the fluctuation region below the critical chemical potential might signal deviations to the classical-field picture which is expected to be accurate for $\tilde{g} \ll 1$ [6,7]. Theoretically this deviation could be addressed using quantum Monte Carlo methods [28,29].

In conclusion, we have presented a method to determine the EoS of a scale-invariant fluid. This method does not rely on thermometry of individual images, nor on the precise calibration of the detectivity, and it leads to a strong reduction of the noise level in the measurement. We have applied it to the case of a weakly interacting Bose gas and obtained its EoS with a precision of a few percent, in excellent agreement with the theoretical prediction

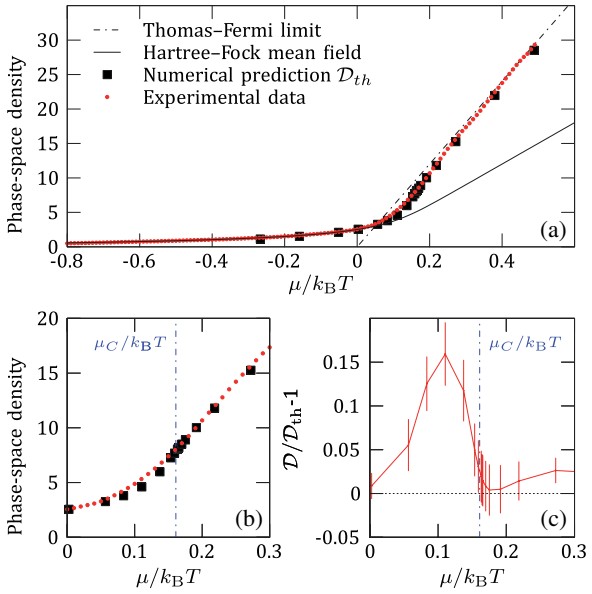

FIG. 3 (color online). (a) Equation of state of the 2D Bose gas, determined with Eqs. (4) and (5) (red points), with a detailed view of the critical region around the BKT transition (blue dash-dotted line) in (b). Statistical error bars are too small to be shown on these plots. We show, for comparison, the classical-field Monte Carlo prediction $\mathcal{D}_{\rm th}$ [7] in black squares, the Thomas-Fermi limit in the black dash-dotted line, and the Hartree-Fock mean-field theory in the black solid line. We provide a quantitative estimate of the difference between measurement and prediction in (c). There, we plot $\mathcal{D}/\mathcal{D}_{\rm th} - 1$, where zero indicates perfect agreement. The error bars result from a bootstrap analysis of the experimental data.

obtained from a classical Monte Carlo simulation. Using the response of the gas to a gauge field, originating, for example, from a rotation, this method could be extended to access the superfluid fraction of the gas along the lines proposed in [1]. In principle, this method is not limited to scale-invariant systems and could be extended to any situation described by two independent dimensionless parameters, such as the zero temperature limit of the Fermi gas, either for a spin-balanced gas with varying interactions [3] or for a unitary spin-imbalanced Fermi gas [30].

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[23] In our case, the compressibility is given by $\kappa = X_1/(n^2h^2/m)$ and the pressure by $P = X_{-1}n^2h^2/m$.
[24] We extract data points with $X_{-1} < 2.5$ ($X_{-1} > 2.5$) from high (low) intensity imaging.
[25] This factor is taken into account in Eq. (1) by $E = \beta(\hbar^2/m)n$. The definition of X_ν is unchanged.
[26] The error bar on this value is calculated through a bootstrap analysis. The result is consistent with our (less precise) previous estimate for the same setup, $\beta = 0.40(2)$, which was based on a different method [14].
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