

Critical Point of a Weakly Interacting Two-Dimensional Bose Gas

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We study the Berezinskii-Kosterlitz-Thouless transition in a weakly interacting 2D quantum Bose gas using the concept of universality and numerical simulations of the classical $|\psi|^4$ model on a lattice. The critical density and chemical potential are given by relations $n_c = (mT/2\pi\hbar^2)\ln(\xi\hbar^2/mU)$ and $\mu_c = (mTU/\pi\hbar^2)\ln(\xi_\mu\hbar^2/mU)$, where T is the temperature, m is the mass, and U is the effective interaction. The dimensionless constant $\xi = 380 \pm 3$ is very large and thus any quantitative analysis of the experimental data crucially depends on its value. For ξ_μ our result is $\xi_\mu = 13.2 \pm 0.4$. We also report the study of the quasicondensate correlations at the critical point.

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An accurate microscopic expression for the critical temperature of the Berezinskii-Kosterlitz-Thouless (BKT) transition [1] has been a weak point of the theory of weakly interacting two-dimensional (2D) Bose gas. The theory of Ref. [2] (see also [3,4] and analysis below) suggests that the critical density of the BKT transition in the weakly interacting system reads (we set $\hbar = 1$)

$$n_c = \frac{mT}{2\pi} \ln \frac{\xi}{mU}. \quad (1)$$

The relation between the effective long wavelength interaction U and microscopic potential $V(r)$ is provided by the 2D quantum scattering theory with self-consistent momentum cutoff of logarithmic renormalization at the inverse interparticle separation [2]

$$U = \frac{V_0}{1 + (mV_0/4\pi)\ln(1/n_c d^2)}, \quad (2)$$

where V_0 is the zero-momentum Fourier component of $V(r)$, and d is the potential radius. In quasi-2D systems V_0 and d depend also on the confining geometry and the 3D scattering length [3,5] (after projecting the third direction out).

Unfortunately, the value of ξ is outside existing analytical treatments since it is related to the system behavior in the fluctuation region where perturbative expansions in powers of U do not work. With unknown ξ , one finds Eq. (1) rather inaccurate unless mU is exponentially small. Moreover, as we find in this Letter, the value of ξ is very large: $\xi \approx 380$. In this connection we mention that the answer for the extremely dilute system [when $mU \approx 4\pi/\ln(1/n_c d^2)$],

$$n_c = \frac{mT}{2\pi} [\ln(\xi/4\pi) + \ln \ln(1/n_c d^2)], \quad (3)$$

never acquires its known limiting form [4], $n_c \approx (mT/2\pi)\ln \ln(1/n_c d^2)$, in realistic systems, because it is impossible to have $\ln(1/n_c d^2) \gg \xi/4\pi \approx 30$. Thus for all experimentally available up to date (quasi-)2D weakly interacting Bose gases [6,7] the *quantitative* analysis of the data for the critical ratio n_c/T_c in terms of microscopic

parameters requires a precise value of ξ . In the system of spin-polarized atomic hydrogen on helium film [6], the value of mU is of order unity [3]; in the recently created quasi-2D system of sodium atoms [7], mV_0 is of order 10^{-2} , according to the formula of Ref. [5].

To quantitatively describe the limit of small U , it is sufficient to solve a classical-field $|\psi|^4$ model with the effective long-wave Hamiltonian [2]

$$H[\psi] = \int \left\{ \frac{1}{2m} |\nabla\psi|^2 + \frac{U}{2} |\psi|^4 - \mu' |\psi|^2 \right\} d\mathbf{r}, \quad (4)$$

where μ' is the chemical potential and ψ is the classical complex field. By replacing the quantum model with the classical one, we stop quantum renormalizations of U by brute force. The justification for this procedure is in the logarithmically slow dependence of U on momentum and can be taken into account *a posteriori*, as U dependence on either density or temperature [2]; see Eq. (2).

In this Letter, we first discuss the origin of relation (1) in the limit of small U and how quantum and classical models relate to each other. Then we present our numeric results (for the critical density, chemical potential, and quasicondensate correlations) obtained by simulations of the 2D $|\psi|^4$ model on a lattice using recently developed Worm algorithm [8] for classical statistical models. We show that quasicondensate correlations are very strong at T_c , in agreement with the experiments on spin-polarized atomic hydrogen [6] and quantum Monte Carlo simulations [9].

Simple order-of-magnitude analysis of Eq. (4) allows us to write a generic formula for the critical point in a weakly interacting 2D $|\psi|^4$ model. The routine itself is analogous to the 3D case (see, e.g., [10,11]), but final results naturally reflect specific properties of 2D systems. We begin with introducing the mode-coupling momentum, k_c , that characterizes the onset of strong nonlinear coupling between long-wave harmonics of $\psi(\mathbf{r})$ (harmonics with $k \gg k_c$ are almost free). This momentum is just the inverse of the *healing* length, or vortex core radius, r_c [1]. We denote by \tilde{n} the contribution to the total density due to strongly coupled harmonics and introduce the renormalized chemical

potential

$$\tilde{\mu} = \mu' - 2U \int_{k > k_c} n_k^{(\text{ideal})} d^2k / (2\pi)^2 \quad (5)$$

by subtracting the mean-field contribution of noninteracting high-momentum harmonics. Here $n_k = \langle |\psi_{\mathbf{k}}|^2 \rangle$, and $\langle \dots \rangle$ stands for the statistical average.

The Nelson-Kosterlitz formula [12]

$$n_s = \frac{2mT}{\pi} \quad (6)$$

provides an estimate for \tilde{n} since it is intuitively expected that $\tilde{n} \sim n_s$. An independent estimation of the fluctuation region parameters derives by equating all three terms in Eq. (4),

$$k_c^2/m \sim |\tilde{\mu}| \sim \tilde{n}U, \quad (7)$$

and relating $\tilde{n} \sim \sum_{k < k_c} n_k \sim k_c^2 n_{k_c}$ to the renormalized chemical potential by using $T/|\tilde{\mu}|$ in place of the occupation number n_{k_c} . By definition, k_c separates strongly coupled and free harmonics, and thus $n_{k_c} \sim T/[k_c^2/2m - \tilde{\mu}] \sim T/|\tilde{\mu}|$. The order-of-magnitude estimations are (at $T = T_c$)

$$\tilde{n} \sim mT, \quad (8)$$

$$k_c \sim m(UT)^{1/2}, \quad (9)$$

$$\tilde{\mu} \sim UmT. \quad (10)$$

We are now in a position to derive Eq. (1). In 2D the main contribution to the particle number integral $n = \int n_k d^2k / (2\pi)^2$ comes from large momenta between k_c and some model-dependent ultraviolet scale k_* . For classical lattice models it is given by the inverse lattice spacing, $k_* \sim 1/a$; in the continuous quantum system $k_* \sim \sqrt{mT}$ is the thermal momentum. At $k_c \ll k \ll k_*$ we have $n_k \approx 2mT/k^2$, and thus we can write

$$n_c = \frac{mT}{2\pi} \ln(Ck_*^2/k_c^2), \quad (11)$$

where C is some constant. Critical density, Eq. (1), for the quantum Bose gas is obtained by substituting $Ck_*^2/k_c^2 \equiv \xi mT/m^2UT = \xi/mU$.

The dependence on the ultraviolet cutoff reflects differences between *ideal* systems, while the long-wave behavior of all weakly interacting $|\psi|^4$ theories is universal. This fact allows one to relate results for different models by adding/subtracting noninteracting contributions; i.e., up to higher order corrections in U the difference between models \mathcal{A} and \mathcal{B} is given by $(n_c^{(\mathcal{A})} - n_c^{(\mathcal{B})}) = \int [n_k^{(\text{ideal } \mathcal{A})} - n_k^{(\text{ideal } \mathcal{B})}] d^2k / (2\pi)^2$. In what follows, we denote the classical lattice model with lattice spacing a as system \mathcal{A} and analyze results using

$$n_c^{(\text{lat})} = \frac{mT}{2\pi} \ln \frac{A}{m^2 a^2 UT}. \quad (12)$$

The actual system of interest is the quantum Bose gas, so we add and subtract the corresponding ideal-system contributions to get

$$\ln \frac{A}{\xi m a^2 T} = \frac{1}{2\pi m T} \left(\int_{\text{BZ}} \frac{T d^2k}{E(\mathbf{k})} - \int \frac{d^2k}{e^{k^2/2mT} - 1} \right), \quad (13)$$

where BZ means that the first integral is over the Brillouin zone, and $E(\mathbf{k})$ is the dispersion law for the ideal lattice model such that $E(\mathbf{k} \rightarrow 0) \rightarrow k^2/2m$. [The divergences of the two integrals in Eq. (13) at $k \rightarrow 0$ compensate each other.]

Our simulations were done for the simple square lattice Hamiltonian

$$H = \sum_{\mathbf{k} \in \text{BZ}} [E(\mathbf{k}) - \mu] |\psi_{\mathbf{k}}|^2 + \frac{U}{2} \sum_i |\psi_i|^4, \quad (14)$$

where $\psi_{\mathbf{k}}$ is the Fourier transform of the complex lattice field ψ_i and $E(\mathbf{k}) = [2 - \cos(k_x a) - \cos(k_y a)]/ma^2$ is the tight-binding dispersion law. With this dispersion relation the right-hand side in (13) can be evaluated analytically and we obtain the ‘‘conversion’’ formula

$$\xi = A/16. \quad (15)$$

Since final results for dimensionless constants do not depend on m , T , and a , in numerical simulations we set $a = 1$, $T = 1$, and $m = 1/2$ for convenience.

The above consideration for the critical density can be readily generalized to the critical chemical potential, with the result

$$\mu_c = \frac{mTU}{\pi} \ln \frac{\xi_\mu}{mU}. \quad (16)$$

First, we notice that Eq. (16) immediately follows from Eqs. (10) and (5) because the mean-field term is proportional to $-(mUT/\pi) \ln(mU)$ (we actually deal with exactly the same integral). Since the renormalized value $\tilde{\mu}$ is universal, to account for the difference between the classical and quantum models one has to add and subtract mean-field contributions dominated by the ideal behavior. Thus, if the classical model is analyzed using $\mu_c = (mTU/\pi) \ln[A_\mu/m^2 a^2 UT]$, one has to apply $\xi_\mu = A_\mu/16$ to get the quantum result, Eq. (16).

We now turn to our numerical procedure. To simulate the grand-canonical ensemble corresponding to the Hamiltonian (14) we employ the classical Worm algorithm Ref. [8] that has demonstrated its efficiency for the analogous problem in 3D [11]. The formal criterion of the critical point for the system of linear size L is based on the exact Nelson-Kosterlitz relation (6): We say that the system is at the critical point if its superfluid density, $n_s(L)$, satisfies $n_s(L) = 2mT/\pi$ [$n_s(L)$ has a direct estimator in the Worm algorithm via statistics of winding numbers [8], and its autocorrelation time does not suffer from critical slowing down].

The finite-size scaling of $n_c(L)$ is well known from the Kosterlitz-Thouless renormalization group theory [1]

$$n_c(L) = n_c - \frac{A'mT}{\ln^2[A''Lm(UT)^{1/2}]}, \quad (17)$$

where A' and A'' are dimensionless constants. A similar relation applies also to the critical chemical potential. Equation (17) was used for the finite-size scaling analysis. We found that instead of extrapolating data for each value of U to the $L \rightarrow \infty$ limit independently, a much more efficient procedure is to perform a joint finite- L and finite- U analysis. To this end we heuristically introduce parameters accounting for nonuniversal finite- U corrections by adding linear in U terms to each of the three of the dimensionless constants: $A \rightarrow A + BU$, $A' \rightarrow A' + B'U$, and $A'' \rightarrow A'' + B''U$. We thus have six fitting parameters to describe all our data points [13]. The data for $n_c(U, L)$ and $\mu_c(U, L)$ are presented in Fig. 1. The fitting procedure yields $A = (6.07 \pm 0.05) \times 10^3$, $A_\mu = (211 \pm 6)$,

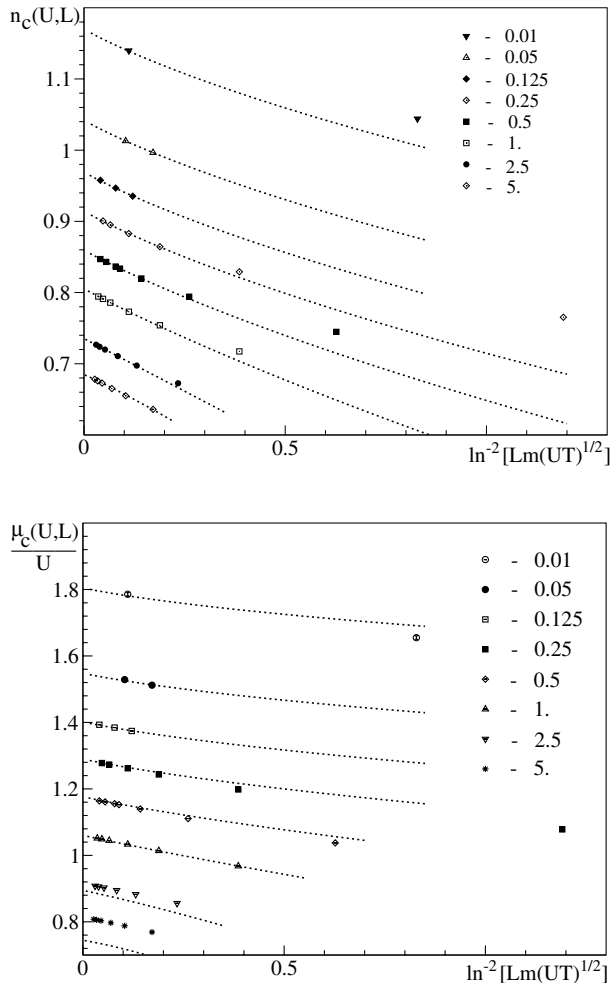


FIG. 1. Critical density and chemical potential for various coupling parameters and system sizes. Typical error bars are much smaller than symbol sizes. The dotted line is the fitting function described in the text.

which, according to Eq. (15), means that

$$\xi = 380 \pm 3, \quad \xi_\mu = 13.2 \pm 0.4. \quad (18)$$

The fit is extremely good: 20 points for the critical density at $U \leq 2.5$ and $Lm(UT)^{1/2} > 15$, each calculated with relative accuracy of order 10^{-4} , are described with the confidence level of 62%.

Experiments on helium films report that the ratio $n_s(T_c)/n_s(0) = n_s(T_c)/n_c = 2mT_c/\pi n_c$ is close to 0.75 [14,15]. Our result for this ratio is given by

$$n_s(T_c)/n_c = \frac{4}{5.94 - \ln(mU)}, \quad (19)$$

and $mU \approx 1.8$ is required to describe helium films, provided the small- U approximation for n_c may be pushed that far [16]. We are not aware of the published data on the critical chemical potential. [For helium and hydrogen films on substrates one has to shift μ_c by the value of the absorption energy (for the delocalized atom, in the case of helium film), $\mu_c \rightarrow \mu_c = E_0 + (mTU/\pi) \ln(\xi_\mu/mU)$. In thermal equilibrium this quantity can be readily measured through the chemical potential of the bulk vapor.]

In the absence of long-range order parameter, 2D systems below T_c are characterized by the local correlation properties of the quasicondensate density, identical to those of a system with genuine condensate [3]. These properties reflect the specific structure of the ψ field:

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \psi_1(\mathbf{r}), \quad (20)$$

$$\psi_0(\mathbf{r}) \approx \sqrt{n_0} e^{i\Phi(\mathbf{r})}, \quad (21)$$

where the quasicondensate density n_0 may be considered as a constant, and ψ_1 is the Gaussian field independent of ψ_0 . Both experiment [6] and model Monte Carlo simulations [9] indicate that in 2D systems with $mU \sim 1$ the quasicondensate correlations appear well above T_c and are pronounced at T_c . Below we show that this is a generic feature of weakly interacting $|\psi|^4$ models.

It is convenient to characterize the quasicondensate properties by the correlator

$$Q = 2\langle |\psi|^2 \rangle^2 - \langle |\psi|^4 \rangle. \quad (22)$$

The Gaussian component of the field obeys the Wick's theorem and does not contribute to Eq. (22). If, for a moment, by ψ_1 we understand short-wave harmonics of ψ , we conclude that only long-wave and strongly nonlinear harmonics with the momenta $k \sim k_c$ contribute to the correlator Q , i.e., $Q \sim \tilde{n}^2$. Thus, we expect that all weakly interacting $|\psi|^4$ models satisfy

$$Q = C_* m^2 T^2 \quad (T = T_c) \quad (23)$$

in the limit of small U , where C_* is a universal constant. By definition, $n_0 = \sqrt{Q}$.

The finite-size and small- U analysis of the data for $Q(U, L)$ was done in complete analogy with previously discussed cases of $n_c(U, L)$ and $\mu_c(U, L)$ (see Fig. 2 and

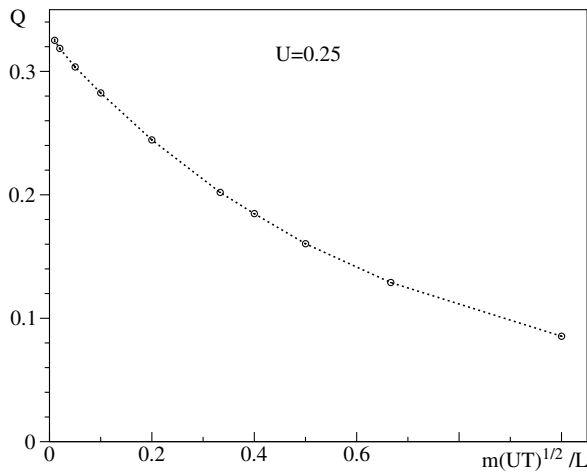


FIG. 2. Quasicondensate correlations as a function of system size. The dotted line is to guide the eye.

Ref. [13]). We found that

$$C_* = 1.30 \pm 0.02. \quad (24)$$

The ratio between $n_0(T = T_c)$ and n_c describes how pronounced are the quasicondensate correlations in the Bose gas at the BKT point:

$$\frac{n_0^{(T=T_c)}}{n_c} = \frac{2\pi\sqrt{C_*}}{\ln(\xi/mU)} = \frac{7.16}{5.94 + \ln(1/mU)}. \quad (25)$$

We see that it is of order unity unless mU is exponentially small. Another interesting ratio is

$$\frac{n_0}{n_s} = \frac{\pi\sqrt{C_*}}{2} \approx 1.79 \quad (T = T_c), \quad (26)$$

which is interaction independent and shows that the superfluid density is substantially smaller than the quasicondensate density at T_c .

Finally, we derive an accurate estimate for the mode-coupling radius r_c . In an ideal system $Q \equiv 0$. Hence, $Q(L)$ should decrease with decreasing L , and for system sizes $L \sim r_c$ it has to drop significantly from its thermodynamic value. We rather formally define r_c from $Q(L = r_c) \approx Q(L \rightarrow \infty)/2$ and from Fig. 2 obtain $r_c \approx 2/m(UT)^{1/2}$.

We conclude by noting that the Nelson-Kosterlitz formula (6) and Eqs. (1), (16), and (23) constitute a complete set of equations which allow us to fully determine system parameters from measurements with independent cross-checks. We are not aware of another study where

dimensionless constants ξ , ξ_μ , and C_* were determined with high precision.

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