Quasicondensation in a two-dimensional interacting Bose gas

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We present a detailed Monte Carlo study of the many-particle density correlations in an interacting two-dimensional (2D) Bose gas, which are responsible for the recombination and spin relaxation rates in real experiments. We confirm that a $1/m!$ effect for local correlators does exist in 2D and can be used for the study of phase transitions. In agreement with a recent experiment [A. I. Safonov *et al.*, Phys. Rev. Lett. **81**, 4545 (1998)], the appearance and growth of quasicondensate fluctuations changes local correlations well before the Kosterlitz-Thouless transition point. Even a moderate interaction considerably reduces the amplitude of the $1/m!$ effect. This conclusion indicates that the enhancement of the $1/m!$ effect observed in the experiment by Safonov *et al.* cannot be ascribed to finite-interaction effects in a purely 2D system.

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The discovery of Bose-Einstein condensation (BEC) in ultracold dilute gases has opened a unique possibility for the study of quantum correlations in these systems. For one thing, it has been observed that inelastic processes are suppressed in the presence of BEC [1], in agreement with theoretical predictions [2]. In a three-dimensional (3D) gas at low temperature $T \ll T_c$ (T_c is the BEC transition temperature), the m-particle correlator

$$K_m = n^{-m}\langle[\Psi^\dagger(\mathbf{0},0)]^m[\Psi(\mathbf{0},0)]^m\rangle \tag{1}$$

is reduced by a factor of $1/m!$ as compared to its value at $T > T_c$ [2]. Here Ψ is the Bose field operator and n is the gas density. This result is exact for the ideal gas, and interaction corrections are small in the gas parameter. In particular, the rate of three-body recombination, $W_3 \sim K_3$, must drop by ~ 6 times [2].

In systems with reduced dimensionality (e.g., in $d=2$) at any finite T the condensate density is zero, and the question of the $1/m!$ effect is not at all obvious. The theory of this effect in 2D was presented in Ref. [3]. In the superfluid state of a weakly interacting 2D Bose gas (and well below the fluctuation region) the phase and density correlation lengths, R_c and r_c, have different scales: $R_c \gg r_c$. This allows the introduction of the notion of a quasicondensate characterized by the value n_0, the amplitude of the one-particle density matrix at intermediate distances, $\rho(r) \approx n_0$ at $r_c \ll r \ll R_c$, where

$$\rho(\mathbf{r}) = \langle\Psi^\dagger(\mathbf{r},0)\Psi(\mathbf{0},0)\rangle. \tag{2}$$

The local properties of the quasicondensate are identical to those of the genuine condensate, which justifies the $1/m!$ effect. However, in contrast to the 3D case, a nonzero n_0 in 2D is due only to finite interparticle interaction, which, in its turn, can reduce the drop of K_m. Another complication is associated with the fact that the fluctuation region near the Kosterlitz-Thouless (K-T) temperature T_c (or n_c if temperature is kept fixed) is rather wide, especially in view of the fact that the gas parameter is usually not so small in 2D. Thus, one may observe a rather broad transformation of local correlation functions near T_c or n_c, which falls outside existing analytic treatments.

Since the $1/m!$ effect itself can be used for detection and study of phase transitions in the interacting 2D system through the rate of inelastic processes, two experimental studies have been attempted in spin-polarized hydrogen on a helium film [4,5]. The advantage of such measurements in comparison with the standard search for the K-T transition in torsion-type experiments [7] is that they are not influenced by the substrate and are quasistatic. To ensure that specific 2D features do not pose any problems in this approach we have performed a direct *ab initio* calculation of K_2 and K_3 correlators (related to the spin relaxation and three-body recombination rates) using quantum Monte Carlo (MC) simulations. We found that the $1/m!$ effect is clearly observable.

Recently it was announced [6] that spin-polarized hydrogen on a helium surface undergoes a phase transition; the conclusion is based on the significant drop of the three-particle recombination rate as a function of n at fixed T. There are two intriguing features in the experiment [6] which need theoretical understanding. First, the decrease of the recombination rate starts well before the K-T transition point. The reason is an anomalously broad fluctuation region above T_c (where the superfluid density $n_S=0$) with strong quasicondensate fluctuations, as follows from the results of our calculations. We have also found that the amplitude of the $1/m!$ effect is *suppressed* by interparticle interactions, and the "ideal" value $1/m!$ is realized only in the limit of vanishing interaction. In this connection the result of Ref. [8] must be considered as incorrect and misleading, since it predicts an *enhanced* decrease of W_3 (by a factor of 1/400).

The other nontrivial feature of the data [6] is that W_3 drops more than $3!$ times. As mentioned already, such a decrease of W_3 in a purely 2D system *cannot* be explained by finite-interaction effects. However, due to the delocalization perpendicular to the surface, this system is only *quasi*-2D, the delocalization length increasing with density [9]. The effect of delocalization itself may result in a very strong suppression of W_3, as predicted in Ref. [9]. We do not see another alternative to understand the experimental data.

For realistic interatomic potentials and particle densities the fluctuation region is too wide to allow reliable analytic treatment of correlation functions. We thus attempted a MC simulation of the 2D Bose gas in the grand canonical ensemble, by varying the degeneracy parameter $n/(mT)$ (where m is the atom mass) through the chemical potential μ (in the experiment [6] the surface density is controlled by μ of the bulk buffer gas).

Our MC simulation is based on the recently developed continuous-time Worm algorithm [10], which is extremely effective in calculating Green functions (at any temperature) and is free of systematic errors. Thus apart from the local correlation functions, Eq. (1), we also evaluate the one-particle density matrix $\rho(r)$, Eq. (2).

We use a model Hamiltonian on the square lattice [11]

$$H=-t\sum_{\langle ij\rangle} a_i^\dagger a_j+\frac{U}{2}\sum_i n_i^2, \quad n_i=a_i^\dagger a_i, \tag{3}$$

where $a_i^\dagger$ creates a boson on site *i*, and $\langle ij\rangle$ stands for pairs of nearest neighbor sites. The particular form of the short-range interaction is not important in the dilute limit, and we restrict ourselves to the on-site Hubbard repulsion *U*.

To ensure that the underlying lattice plays no role, we choose parameters so that the characteristic one-particle energies are much less than the bandwidth $W=8t$, i.e., we require $T,U\ll 8t$. Though the variable $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$ is essentially discrete, in the quasicontinuous case, the density matrix $\rho(r)$ is a smooth function of $r=|\mathbf{r}_{ij}|$.

At the band bottom we may employ the quadratic expansion $\epsilon_k=k^2/2m$ for the dispersion law with $m=\hbar^2/(2ta^2)=1/2$ (in what follows we use units such that $\hbar=1$, $t=1$, and $a=1$). The strength of the interaction is naturally characterized by the relative depletion of the condensate density at zero temperature $\xi=(n-n_0)/n$, which can be easily derived in the framework of the standard Bogoliubov transformation:

$$\xi=U/8\pi. \tag{4}$$

We will study the case when ξ is small. However, U will be strong enough to see the effect of interparticle interaction on local correlators.

To estimate the lower boundary for the critical density we employ the universal relation for the K-T temperature [12], $T_c=\pi n_S^-/2m=\pi n_S^-$, where n_S^- is the superfluid density at $T\to T_c-0$. Thus, at a fixed temperature

$$n_c>n_S^-=T/\pi. \tag{5}$$

For $T=0.2$ and $T=0.1$ we have $n_s^-\approx 0.064$ and $n_s^-\approx 0.032$, respectively. Note that for both the above-mentioned temperatures (for which we will present below our numerical results) the K-T transition occurs at relatively low densities.

A typical evolution of $\rho(r)$ with increasing degeneracy is presented in Fig. 1. The curves are obtained for a lattice with $L\times L=80^2$ sites (we use periodic boundary conditions). In the normal state [Fig. 1(a)] there is only one characteristic length scale—the thermal de Broglie wavelength, and $\rho(r)$ decays exponentially with *r*. In Figs. 1(c),(d) we see a well-developed quasicondensate state, characterized by two different length scales—after a fast short-range decrease to a certain value (the quasicondensate density n_0), ρ continues to decay very slowly. The case shown in Fig. 1(b) is an intermediate one. Though there is no pronounced bimodal shape yet, the decay of ρ at larger *r*'s is anomalously slow. This type of behavior is observed in a rather wide range of variation of the degeneracy parameter (the fluctuation region).

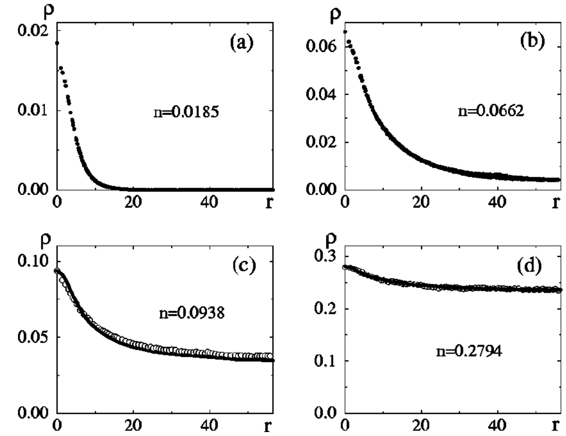

FIG. 1. Evolution of one-particle density matrix with density. $T=0.2$, $U=1.0$. Solid curves in (c) and (d) are obtained from Eqs. (6)–(9), and contain *no* fitting parameters.

Away from the fluctuation region (at $n>n_c$) there exists an analytic representation for $\rho(r)$ [13]. Within Popov's functional-integral approach [14] one obtains the following set of coupled equations that has to be solved self-consistently for $\rho(r)$, n_0, and the elementary excitation spectrum $E(k)=\sqrt{\epsilon(k)[\epsilon(k)+2n_0\tilde{U}]}$:

$$\rho(r)=e^{-\Lambda(r)}\tilde{\rho}(r), \quad n_0=\tilde{\rho}(r\to\infty); \tag{6}$$

$$\Lambda(r)=\int\frac{d\mathbf{k}}{(2\pi)^2}[1-\cos(\mathbf{k}\cdot\mathbf{r})]\frac{\tilde{U}}{E(k)}\nu(k), \tag{7}$$

$$\tilde{\rho}(r)=n-\int\frac{d\mathbf{k}}{(2\pi)^2}[1-\cos(\mathbf{k}\cdot\mathbf{r})]\left\{\frac{\epsilon(k)+n_0\tilde{U}-E(k)}{2E(k)}+\frac{\epsilon(k)\nu(k)}{E(k)}\right\}. \tag{8}$$

Here $\nu(k)=\{\exp[E(k)/T]-1\}^{-1}$ is the Bose function,

$$\tilde{U}=\frac{U}{1+(mU/2\pi)\ln(r_c/d_0)} \tag{9}$$

is the effective interaction, and d_0 is a cutoff for distance. Expression (9) implies that $d_0\ll r_c$. When the degeneracy parameter is on the order of unity or larger, to a good approximation one may set $r_c\sim n^{-1/2}$ in Eq. (9).

In our model, d_0 is just the intersite distance. The function $\tilde{\rho}(r)$ describes short-range decay of the density matrix to the

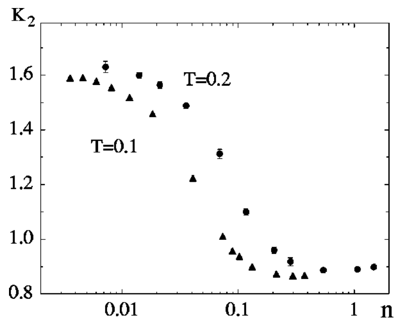

FIG. 2. Two-particle density correlator as a function of density at $U=0.4$.

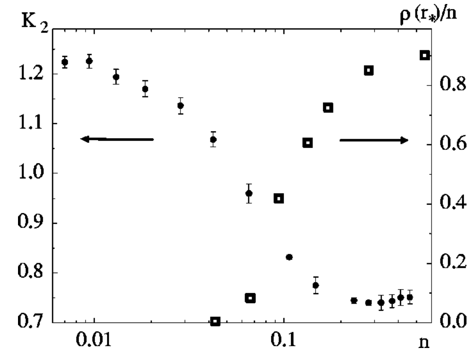

FIG. 4. $K_2(n)$ and $\rho(r_*,n)$ curves for $U=1.0$, $T=0.2$, demonstrating decoupling of short-range and long-range correlation properties (here $r_*=40$).

quasicondensate density value n_0. The long-range decay of ρ is described by the slowly growing exponent $\Lambda(r)$ associated with phase fluctuations. For $n>n_c$, we observe a remarkably good agreement between $\rho(r)$ calculated from Eqs. (6)–(9) and our MC results; the agreement becomes progressively better away from the fluctuation region [see Figs. 1(c),(d)].

We now turn to the local density correlators Eq. (1). In Figs. 2 and 3 we present the data for K_2 and K_3 as functions of density n for two temperatures $T=0.2$ and $T=0.1$, at $U=0.4$ (in units of t). (The system size ranges from 80^2 for higher n's up to 300^2 for lower n's.) We see a pronounced strong decrease of K_m when the density varies from $n \ll n_c$ to $n \gg n_c$. The most striking result is the very broad crossover region. Both correlators start to decrease at densities well below n_c.

It is important to verify that our results are not artifacts of finite-size effects since for finite L there exists a considerable fraction of *genuine* condensate even at *finite* temperature [this fraction is given by $\rho(r_*)$, where $r_* \sim L$], and thus changes in local correlators could be due to global condensation (as in the 3D case) rather than quasicondensation. We checked explicitly that the point $U=1.0$, $n=0.04$, $T=0.2$, where there is already a pronounced decrease of K_2 and K_3, is not sensitive, within the error bars, to the system size for $L=60$, 100, and 200. Also, we proved that at this point the value of $\rho(r_*)$ is not a relevant quantity, being very small at our largest available L's (see Fig. 4). Most convincingly, in Fig. 4 we see that the crossover in K_2 starts well before $\rho(r_*)$ becomes appreciable.

The decrease of K_m in the region $n<n_c$ is indicative of strong quasicondensate fluctuations in the normal state. In principle, this behavior is not unexpected, since n_0 is not directly related to the superfluid density n_S. If the concentration of vortices is small in the fluctuation region $n<n_c$, the quasicondensate can survive, being related to the short-range correlation properties. The variation of n_0 thus has a form of crossover rather than a transition.

In the limit of very small (but finite) interaction, the K_m's should change their values from $m!$ to 1 throughout the transition. The data presented in Figs. 2 and 3 demonstrate two characteristic plateaus at $n \ll n_c$ and $n \gg n_c$, the ratio between the two (at $T=0.1$) being equal to ≈ 4.6 for K_3 and to ≈ 1.85 for K_2, and smaller than $m!$ The absolute values of the correlators are also considerably smaller than in the case of negligibly small U. We thus conclude that even $U=0.4$ is not small enough to yield an idealized picture. Figure 5 clearly demonstrates decreasing amplitudes of the 1/2 effect with increasing interaction. A similar picture was also observed for the correlator K_3. At this point we note that the $K(U)$ dependence is not universal and can be sensitive to the particular form of the interaction potential. It is crucial, however, that we observe *weakening* of the $1/m!$ effect with increasing U.

As mentioned already, the three-body dipole recombination rate W_3 (proportional to K_3) of spin-polarized atomic hydrogen adsorbed on the surface of superfluid helium was found to fall drastically with increasing n, and the decrease of W_3 started well before the critical point n_c is reached [6]. This remarkable result is in qualitative agreement with our MC simulations. Unfortunately, direct quantitative compari-

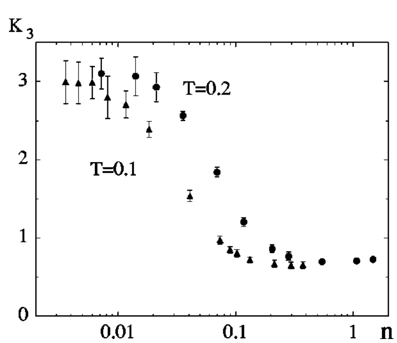

FIG. 3. Three-particle density correlator as a function of density at $U=0.4$.

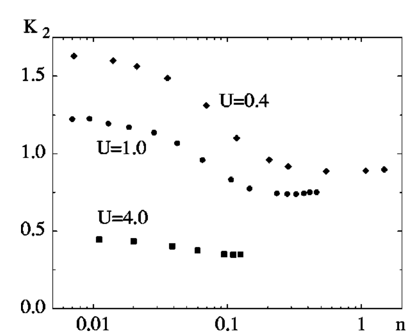

FIG. 5. $K_2(n)$ curves for various coupling strengths U, calculated at $T=0.2$.

son is not possible because hydrogen atom delocalization perpendicular to the surface is density dependent. Indeed, n cannot exceed some maximum value $n_{\max}$. When $n \to n_{\max}$ the absorption energy goes to zero and the hydrogen atom wave function in the direction perpendicular to the surface essentially changes its form due to collective effects [9]. This specific restructuring of the wave function leads to an additional drop of W_3 [through the density-dependent factor $\alpha(n)$ in $W_3 = \alpha K_3$]. As a result, if n_c is close to $n_{\max}$, the observed rate W_3 may drop by a factor much larger than 6 (up to 40) [9]. As far as we can see, this is the only possible explanation for the measured ratio $W_3(n \ll n_c)/W_3(n \gg n_c) > 6$ [6].

Summarizing, we studied quasicondensation in a 2D interacting Bose system at finite T including the wide fluctuation region around T_c. We traced the evolution of the one-particle density matrix and local correlators with increasing degeneracy parameter. We found that quasicondensate features appear far away from the K-T transition point. The effect of qusicondensation on local correlation properties is clearly seen in this region, but its strength is rather sensitive to the interparticle interaction.

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