Quasicondensation in 2D Interacting Bose Gas: Quantum Monte Carlo Study

Yu. Kagan\textsuperscript{1,3}, V.A. Kashurnikov\textsuperscript{2}, A.V. Krasavin\textsuperscript{2}, N.V. Prokof'ev\textsuperscript{1}, and B.V. Svistunov\textsuperscript{1,3}

\textsuperscript{1} Russian Research Center “Kurchatov Institute,” 123182 Moscow, Russia
\textsuperscript{2} Moscow State Engineering Physics Institute, 115409 Moscow, Russia
\textsuperscript{3} Institute for Theoretical Physics, UCSB, Santa Barbara, CA 93106

We present a detailed Monte Carlo study of correlations in an interacting two-dimensional Bose gas. The data for one-particle density matrix in coordinate representation are compared to the results for the local many-particle density correlators, which are responsible for the recombination rate in real experiments. We found that the appearance and growth of quasicondensate fluctuations changes local correlations between the particles well before the Kosterlitz-Thouless transition point. The amplitude of the \(1/m\)-effect is very sensitive even to a rather moderate interaction, and is considerably smaller than its limiting value.

PACS numbers: 03.75.Fi, 05.30.Jp, 67.65.+z

The discovery of Bose-Einstein condensation (BEC) in ultra-cold dilute gases has opened a unique possibility for the study of quantum correlations in these systems. For one thing, it was observed that inelastic processes are suppressed in the presence of BEC\textsuperscript{3}, in agreement with theoretical predictions\textsuperscript{2}. In the 3D gas at low temperature \(T < T_c\) (\(T_c\) is the BEC transition temperature), the \(m\)-particle correlator

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

is reduced by a factor of \(1/m!\) as compared to its value at \(T > T_c\)\textsuperscript{3}. Here \(\Psi\) 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 (which is proportional to \(K_3\)) must drop by \(\sim 6\) times\textsuperscript{2}, as was indeed measured in Ref.\textsuperscript{4}.

In systems with reduced dimensionality (e.g., in \(d = 2\)) at any finite \(T\) the condensate density is zero, and the question of \(1/m!\)-effect is not at all obvious. On another hand, below Kosterlitz-Thouless (K-T) temperature \(T_c\) 2D system becomes superfluid due to long-range phase coherence. In the superfluid state one finds that phase and density correlation lengths, \(R_c\) and \(r_c\), may have different scales (\(R_c \gg r_c\)), which allows to introduce the notion of quasicondensate characterized by the value \(n_0\), the amplitude of the one-particle density matrix \(\rho(r)\) at intermediate distances \(r_c \ll r \ll R_c\)

\[ \rho(r) = \langle \Psi^\dagger(r,0)\Psi(0,0) \rangle. \quad (2) \]

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, non-zero \(n_0\) in two dimensions is only due to finite interparticle interaction, which, in its turn, reduces the drop of \(K_m\). Another complication is associated with the fact that fluctuation region near \(T_c\) (or \(n_c\) if temperature is kept fixed) is rather wide. Also, the gas parameter is usually not so small in 2D. Thus, one may observe rather broad transformation of local correlation functions near \(T_c\) or \(n_c\).

The \(1/m!\)-effect itself may be used for the detection and study of BEC. So far experimental attempts to create 2D waveguides for ultra-cold neutral atoms in specially arranged laser and/or magnetic fields (see, e.g., Refs.\textsuperscript{4,5} and Refs. therein) did not succeed in getting necessary conditions for BEC. Another promising system is spin-polarized hydrogen on helium film\textsuperscript{6}. Small binding energy (\(\sim 1\) \(K\)), and strong delocalization perpendicular to the film allow to consider the in-plane motion of hydrogen as free. Recently it was announced\textsuperscript{7} that the system undergoes BEC phase transition as the surface density is increased; the conclusion being based on the significant drop of the three-particle recombination rate. The advantage of such measurements in comparison with the standard search for the K-T transition in torsion-type experiments\textsuperscript{8} is that they are not influenced by the substrate and are quasistatic.

For realistic interatomic potentials and particle densities the fluctuation region is too wide to allow adequate analytic treatment of correlation functions. We thus attempted quantum Monte Carlo (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 \(\mu\). Note that experiments with spin-polarized hydrogen on helium surface are done in the same setup, since surface density is controlled by \(\mu\) of the bulk buffer gas. Surprisingly enough, under the same conditions the theory of Ref.\textsuperscript{9} predicts the decrease of \(K_3\) by a factor of 400! The results presented below unambiguously prove that the theory of Ref.\textsuperscript{9} is in error.

Our MC simulation is based on the recently developed continuous-time Worm algorithm\textsuperscript{10}, which is extremely effective in calculating Green functions (at any temperature), and is free of systematic errors. Thus apart from local correlation functions Eq.\textsuperscript{11}, we also evaluate the one-particle density matrix \(\rho(r)\) Eq.\textsuperscript{12}.

We start with the definition of the model Hamiltonian on the square lattice:

\[ H = -\sum_{\langle ij\rangle} J \Psi_i^\dagger \Psi_j + \mu \sum_i \Psi_i^\dagger \Psi_i, \]
\[ H = -t \sum_{<ij>} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i^2, \quad n_i = a_i^\dagger a_i, \quad (3) \]

where \( a_i^\dagger \) creates a boson on site \( i \), and \( <ij> \) stands for the 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 underlying lattice plays no role, we choose parameters so that characteristic one-particle energies are much less than the bandwidth \( W = 8t \), i.e., we require \( T, U < 8t \). Though the variable \( r_{ij} = |r_i - r_j| \) is essentially discrete, in the quasi-continuous case, the density matrix \( \rho(r) \) is a smooth function of \( r = |r_{ij}| \).

At the band bottom we may employ 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 interaction is naturally characterized by 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:

\[ \xi = U/8\pi. \quad (4) \]

On one hand, we will study the case when \( \xi \) is small. On the other hand, the parameter \( U \) will be strong enough to see the effect of interparticle interaction on local correlators \( K_m \).

To estimate the critical density we employ the universal relation for the K-T temperature \( T_c = \pi n_0^{-}/2m = \pi n_S^{-} \), where \( n_S^{-} \) is the superfluid density at \( T \to T_c - 0 \). At a fixed temperature \( T \) the critical value of \( n_S^{-} \) is given by

\[ n_S^{-} = T/\pi. \quad (5) \]

For \( T = 0.2 \) and \( T = 0.1 \) we have \( n_S^{-} \approx 0.064 \) and \( n_S^{-} \approx 0.032 \), correspondingly. Though the critical density \( n_c > n_S^{-} \), the difference is normally not large. Hence, for an estimate of \( n_c \) one can use \( n_S^{-} \) \( (3) \). Note that for both 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 the lattice with \( L \times L = 80^2 \) sites (we use periodic boundary conditions). In a normal state \([Fig. 1(a)]\) there is only one characteristic length-scale - 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 fast short-range decrease to a certain value (quasicondensate density \( n_0 \), \( \rho \) 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 \( \rho \) at larger \( r \)'s is anomalously slow. This type of behavior is observed in a rather wide range of variation of the degeneracy parameter (fluctuation region).

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

\[ \tilde{\Lambda}(r) = \int \frac{dk}{(2\pi)^2} \left[ 1 - \cos(kr) \right] \frac{\tilde{U}(k)}{E(k)}, \quad (7) \]

\[ \tilde{\rho}(r) = n - \int \frac{dk}{(2\pi)^2} \left[ 1 - \cos(kr) \right] \times \left\{ \frac{e(k) + n_0\tilde{U} - E(k)}{2E(k)} + \frac{e(k)v(k)}{E(k)} \right\}. \quad (8) \]

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

\[ \tilde{U} = \frac{U}{1 + (mU/2\pi) \ln(1/d_0k_c)} \quad (9) \]

is the effective interaction, \( d_0 \) is a cutoff for distance, and \( k_c \) is a typical momentum. Expression \( \Lambda(r) \) implies that \( d_0k_c \ll 1 \). When the degeneracy parameter is on the order of unity or larger, to a good approximation one may set in Eq. \( (4) \) \( k_c \sim \sqrt{n} \). 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 quasicondensate density value \( n_0 \). The long-range decay of \( \rho \) is described by slowly growing exponent \( \Lambda(r) \). 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 \( \langle 1 \rangle \). 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 \( U = 0.4 \). [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 density varies from \( n \ll n_c \) to \( n \gg n_c \). The most striking result is the very broad cross-over 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. (Almost by definition, this fraction is given by \( \rho(r_*) \), where \( r_* \sim L \).) Hence, the change in local correlators could be due to global condensation (like in 3D case), rather than quasicondensate. 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 cross-over rather than a transition. In the limit of very small (but finite) interaction \( K_m \)'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 \( \approx 4.6 \) for \( K_3 \), and to \( \approx 1.85 \) for \( K_2 \), and smaller than \( m! \). The absolute values of 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 yeald an idealized picture. Fig. 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 \( K(U) \) dependence is not universal and can be sensitive to a particular form of the interaction potential. It is crucial however
that we observe weakening of the $1/n!$-effect with increasing $U$, which is in a sharp contradiction with Ref. [11] predicting an enormous enhancement of the effect.

![Image](image_url)

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

The three-body dipole recombination rate $W_3$ [15] (proportional to $K_3$) of spin-polarized atomic hydrogen, adsorbed on the surface of superfluid helium was measured recently in Ref. [8]. Hydrogen dynamics perpendicular to the surface is quantized since there is only one localized state, and at relevant temperatures ($\sim 200 mK$) the system may be considered as purely two-dimensional. In these experiments $W_3$ was studied as a function of surface density $n(\mu)$. It was found that recombination rate falls drastically with increasing $n$, and the decrease of $W_3$ starts well before the critical point $n_c$ is reached. This remarkable result is in qualitative agreement with our MC simulations. Unfortunately, direct quantitative comparison is not possible because hydrogen atom delocalization perpendicular to the surface is density dependent. Indeed, $n$ cannot exceed some maximum value $n_m$. When $n \to n_m$ 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 [10]. This specific restructuring of the wavefunction leads to the 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 $n_m$, the observed rate $W_3$ may drop by a factor much larger than 6 (up to 40) [14]. As far as we can see, this is the only possible explanation for the measured ratio $W_3(n \ll n_c)/W_3(n \gg n_c) > 6$ [8].

Summarizing, we studied quasicondensation in a two-dimensional interacting Bose system in a rather interesting and experimentally important regime when interaction is not very small. We traced the evolution of 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 quasicondensation on local correlation properties – the main phenomenon directly relevant to the experiment – is clearly seen in this region, but its strength is rather sensitive to the interparticle interaction.

This work was supported by the Russian Foundation for Basic Research (under Grant No. 98-02-16262) and by the Grant INTAS-97-0972 [of the European Community].

[1] E.A. Burt, R.W. Christ, C.J. Myatt, M.J. Holland, E.A. Cornell, and C.E. Wieman, Phys. Rev. Lett. 79, 337 (1997).
[2] Yu. Kagan, B.V. Svetunov, and G.V. Shlyapnikov, Sov. Phys. - JETP Lett. 42, 209 (1985).
[3] Yu. Kagan, B.V. Svetunov, and G.V. Shlyapnikov, Sov. Phys. - JETP 66, 314 (1987).
[4] Yu.B. Ovchinnikov, I. Mlnek, and R. Grimm, Phys. Rev. Lett. 79, 2225 (1997).
[5] E.A. Hinds, M.G. Boshier, and I.G. Hughes, Phys. Rev. Lett. 80, 645 (1998).
[6] A.I. Safonov, S.A. Vasilyev, I.S. Yasnikov, I.I. Lukashevich, and S. Jaakkola, Sov. Phys. - JETP Lett. 61, 1032 (1995).
[7] A.P. Mosk, P.W.H. Pinkse, M.W. Reynolds, T.W. Hijmans, and J.T.M. Walraven, J. Low Temp. Phys. 110, 199 (1998).
[8] A.I. Safonov, S.A. Vasilyev, I.V. Yasnikov, I.I. Lukashevich, and S. Jaakkola, to be published in Phys. Rev. Lett.
[9] G. Agnolet, D.F. McQueeney, and J.D. Reppy Phys. Rev. B, 39, 8034 (1989).
[10] N.V. Prokof’ev, B.V. Svetunov, and I.S. Tupitsyn, Phys. Lett. A 238, 253 (1998); Sov. Phys. - JETP, 87, 310 (1998).
[11] H.T.C. Stoof and M. Bijlsma, Phys. Rev. E, 47, 939 (1993); Physica B, 194-196, 909 (1994).
[12] D.R. Nelson and J.M. Kosterlitz, Phys. Rev. Lett. 39, 1201 (1977).
[13] B.V. Svetunov, Ph. D. Thesis, Kurchatov Institute, Moscow, 1990.
[14] V.N. Popov, Functional Integrals in Quantum Field Theory and Statistical Physics, (Reidel, Dordrecht, 1983), Chap. 6.
[15] Yu. Kagan, I.A. Vartanyants, and G.V. Shlyapnikov, Sov. Phys. - JETP, 54, 590 (1981).
[16] Yu. Kagan, N.A. Glukhov, B.V. Svetunov, and G.V. Shlyapnikov, Phys. Lett. A 135, 219 (1989).