Quantum Monte Carlo study of a one-dimensional phase-fluctuating condensate in a harmonic trap

C. Gils,1 L. Pollet,1 A. Vernier,2 F. Hebert,2 G.G. Batrouni,2 and M. Troyer1

1Institut für Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland
2Institute Non-Linéaire de Nice, UMR CNRS 6618, Université de Nice-Sophia Antipolis, 1361 route des Lucioles, F-06560 Valbonne, France

(Dated: June 11, 2018)

We study numerically the low-temperature behavior of a one-dimensional Bose gas trapped in an optical lattice. For a sufficient number of particles and weak repulsive interactions, we find a clear regime of temperatures where density fluctuations are negligible but phase fluctuations are considerable, i.e., a quasicondensate. In the weakly interacting limit, our results are in very good agreement with those obtained using a mean-field approximation. In coupling regimes beyond the validity of mean-field approaches, a phase-fluctuating condensate also appears, but the phase-correlation properties are qualitatively different. It is shown that quantum depletion plays an important role.

PACS numbers: 03.75.Hh, 03.75.Lm, 05.30.Jp

In a spatially homogeneous one-dimensional (1D) gas of bosons, spontaneous symmetry breaking is excluded at all temperatures $T \ll \omega$. Long-range order is absent in this system due to the fluctuations of the phase of the order parameter, as seen in the asymptotic decay of the equal-time single-particle Green’s function (algebraic for $T = 0$ and exponential for $T > 0$). However, analytical studies of trapped 1D Bose gases with a fixed particle number, $N$, reveal new phenomena. For example, the ground state of a noninteracting 1D Bose gas in a harmonic trap with frequency $\omega$ becomes macroscopically populated below a temperature $T_c \simeq N\hbar\omega/\ln(2N)$, i.e., a Bose-Einstein condensate (BEC) exists in the finite system [8]. Several mean-field studies indicate that weak repulsive interactions introduce an additional effect, namely, that fluctuations of the density are suppressed at low temperatures, and a phase-fluctuating condensate, or quasicondensate, appears [9, 10, 11, 12, 13, 14]; for the homogeneous system see [15, 16, 17]. Roughly speaking, this is a regime in temperature where the distribution of particles in space is given by a temperature-independent Thomas-Fermi profile, while thermal fluctuations of the phase are present and lead to a phase-coherence length that is smaller than the condensate cloud. Only below a much lower temperature do phase fluctuations also become negligible and phase coherence extends over the complete condensate cloud. A phase-fluctuating condensate emerges only in low dimensions and has been experimentally observed in sufficiently anisotropic 3D trapping geometries [18].

In this paper, we verify the existence of a 1D quasicondensate, on trapped optical lattices, starting from a microscopic approach whose validity is not restricted to certain parameter regimes. Using quantum-Monte Carlo simulations of the Bose-Hubbard model, we investigate the properties of the phase-fluctuating condensate for various choices of interaction strength and density. For weak interactions, our results are in excellent agreement with mean-field estimates in the continuum [10]. In an intermediate-coupling regime beyond the weakly interacting limit, but not yet in the strong-coupling domain, the quasicondensate regime spreads over an even larger temperature range. Nonetheless, we observe qualitatively different phase-correlation properties which do not follow from existing analytical approaches.

First, we briefly review the notion of a quasicondensate (QC) in a weakly interacting (WI) 1D trapped Bose gas as presented in [18]. In the WI limit, we have $\gamma = mg^2n \ll 1$, where $n$ is the average particle density, $m$ the particle mass, and $g$ the coupling constant of a repulsive contact interaction [17]. In second-quantized representation, the Hamiltonian of the system is given by

$$\hat{H} = \int dz \hat{\psi}^\dagger (z) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_1(z) + \frac{g}{2} \hat{\psi}^\dagger (z) \hat{\psi} (z) \right) \hat{\psi} (z),$$

(1)

where $\hat{\psi} (z)$ is the bosonic field operator and $V_1(z) = m\omega z^2/2$ the external trapping potential centered at the origin. The authors in [18] show that density fluctuations $\langle \delta \hat{n}(z) \delta \hat{n}(\zeta) \rangle$, where $\hat{n}(z) = \hat{\psi} (z) \hat{\psi}^\dagger (z)$, are suppressed for inverse temperatures $\beta > \beta_d = (N\hbar\omega)^{-1}$ (Boltzmann constant $k_B = 1$). The field operator can then be expressed as $\hat{\psi} (z) = \sqrt{\hat{n}(z)} \exp[i\hat{\phi} (z)]$. Thermal fluctuations of the phase are evident from the decay of the one-particle density matrix, or (equal-time) Green’s function, which is obtained as [18]

$$\langle \hat{\psi}^\dagger (z) \hat{\psi} (\zeta) \rangle = \sqrt{\hat{n}(z)\hat{n}(\zeta)} \exp(-\langle \delta \phi_{zz}^2 \rangle/2),$$

(2a)

where $\delta \phi_{zz}^2 = (\phi (z) - \langle \phi (z) \rangle)^2$, and

$$\langle \delta \phi_{zz}^2 \rangle = \frac{4\beta_d \mu_{TF}}{3\beta \hbar \omega} \ln \left( \frac{L_{TF} - z}{L_{TF} + z} \right),$$

(2b)

where $\mu_{TF} = (3N\hbar^2/4)^{1/3} (m\omega^2/2)^{1/3}$ is the chemical potential, and $L_{TF} = \sqrt{2\mu_{TF}/m\omega^2}$ the half size of the...
condensate in the Thomas-Fermi (TF) approximation ($\mu_{TF} \gg \hbar \omega$; see e.g. [19]). For $\beta \to \infty$, it follows from Eq. [23] that $\langle \delta \hat{\phi}_{z}^2 \rangle \to 0$, and thus $G(z,z') \to \sqrt{n(z)n(z')}$, i.e. the system is completely phase coherent.

As is well known [18], the discretization of Eq. [11] yields the Bose-Hubbard model with lattice Hamiltonian

$$\hat{H} = -J \sum_{<j,j'>} (\hat{a}_{j}^{\dagger} \hat{a}_{j'} + \text{H.c.}) + \frac{U}{2} \sum_{j} \hat{n}_{j} (\hat{n}_{j} - 1) + V_{t} \sum_{j} (j - M/2)^2 \hat{n}_{j}, \quad (3)$$

where $\hat{a}_{j}^{\dagger}$ creates a particle at optical lattice site $j$ and $\hat{n}_{j} = \hat{a}_{j}^{\dagger} \hat{a}_{j}$. The number of lattice sites $M$ is chosen such that the occupation at the boundaries of the lattice is zero. We work in units where the lattice spacing and $\hbar^2/2m$ are set to 1. In these units, parameters in Eqs. [11] and [3] are related as follows: $J = 1$, $U = g$, $V_{t} = (\hbar \omega)^2/4$. Our system is defined on an optical lattice, however, in the WI and degenerate limits, the discrete and continuum description of the phase-fluctuating condensate are equivalent [12]. We investigate this model using a worm update quantum Monte Carlo (QMC) method in the canonical ensemble [20]. This nonlocal update scheme allows for an efficient evaluation of the equal-time Green’s function $G(j,j') = \langle \hat{a}_{j}^{\dagger} \hat{a}_{j'} \rangle$. Phase correlation properties are also apparent from the shapes of the momentum profile, $n(k) = \sum_{j,j'} G(j,j') \exp[ik(j-j')]$, and the rescaled Green’s function (phase correlation function), $C(j,j') = G(j,j')/\sqrt{n_{j}n_{j'}}$, where $n_{j} = \langle \hat{n}_{j} \rangle$ is the density distribution. In the WI, TF and mean-field ($N$ large enough) limits, we observe three different regimes in temperature: the thermal regime (TR), the quasicondensate (QC) and the “true condensate” (TC). These regimes are separated by smooth crossovers, which are characterized by the temperatures $1/\beta_{QC}$ and $1/\beta_{TC}$. We discuss the properties of the three regimes and compare our results with the mean-field results listed above. Furthermore, we consider the emergence of the phase-fluctuating condensate depending on the choice of parameters $N$, $U$ and $V_{t}$, including parameter sets that are beyond the WI limit.

In the thermal regime $\beta < \beta_{QC}$, both the density and the phase are governed by thermal fluctuations. Hence, all quantities exhibit a strong temperature dependence. The width of the density profile, $L_{n}(\beta)$ (standard deviation of $n_{j}$), decreases throughout the TR, until it reaches its minimum value $L_{n}^{sat}$ at the inverse temperature $\beta_{QC}$, as shown in Fig. 1. The shape of the density profile is approximately Gaussian, which is expected for high temperatures where the bosonic nature of the particles becomes less relevant [Fig. 1a]. The strong phase fluctuations are seen in the width of the momentum profile, $L_{k}(\beta)$ [standard deviation of $n(k)$], which is much larger than its minimum value $L_{k}^{sat}$ [Fig. 1], as well as in the exponential decay of the Green’s function [Fig. 1a]. We recall that there exists no analytical estimate for $\beta_{QC}$; density fluctuations are merely predicted to become small for $\beta \gg \beta_{q} = (4V_{t}N^2)^{-1/2}$ [17]. For the parameter set in the Figs. 1 we have $\beta_{q} \approx 0.02\beta_{QC}$.

In the quasicondensate ($\beta_{QC} \leq \beta < \beta_{TC}$), the density

![FIG. 1: (Color online) (i) Thermal regime: As a result of both density and phase fluctuations, the widths of the density profile, $L_{n}$, and the momentum profile, $L_{k}$, depend on $\beta$ with $L_{n}(\beta) > L_{n}^{sat}$. (ii) Quasicondensate: Density fluctuations are negligible ($L_{n} = L_{n}^{sat}$). (iii) True condensate: In the Thomas-Fermi (TF) approximation, the number of lattice sites $M > N/2$.](image1)

![FIG. 2: (Color online) $N = 2000$, $U = 0.4$, $V_{t} = 0.3$ ($\gamma = 0.003$). Density fluctuations are suppressed for $\beta \geq \beta_{QC} \approx 0.03$ and the density profiles $n_{j} = \langle \hat{n}_{j} \rangle$ (c) are identical for $\beta \geq \beta_{QC}$ (b)-(d). In (a), the line is a fit to a Gaussian profile, while in (b)-(d) the lines are fits to a TF profile $n_{j}(1 - j^2/L^2)$ where $L = 12.6$ ($L_{TF} = 12.6$). Error bars in the figures are always smaller than the symbol size.](image2)
no longer fluctuates: the density profiles $n_j$ at different temperatures $\beta \geq \beta_{QC}$ are identical and in excellent agreement with a TF inverse parabola shape of half size $L$, where $L$ equals to $L_{TF}$ [Figs. 2(b)-2(d)]. However, thermal fluctuations of the phase are considerable. Thus, the width of the momentum profile, and the phase correlation function still change with decreasing temperature (Fig. 3). Figures 3(b)-3(d) demonstrate that the Green’s function varies substantially for different $\beta \geq \beta_{QC}$, while the density profile $\sqrt{n \rho_{ij}}$ is invariant. We find very good agreement with the mean-field result Eq. (2): the ansatz $\sqrt{n \rho_{ij}} \exp\{-\alpha \ln[(L-j)/(L+j)]\}$, with $\alpha$ a fitting parameter, reproduces $G(0,j)$ (Fig. 3).

At temperatures much lower than $1/\beta_{QC}$, phase fluctuations also become suppressed. Therefore, it is meaningful to introduce a second crossover temperature, $1/\beta_{TC}$, to a phase-coherent regime, the true condensate. We define $\beta_{TC}$ as the temperature where $C(0,0.8L) = \exp(-0.25)$. This definition is somewhat arbitrary, but yields a scale below which the system can safely be considered to be phase-coherent. In addition, it allows for a comparison of analytical and numerical results, with the analytical equivalent of $\beta_{TC}$ being $\beta_{TC} = 4\beta_{HTF} \ln(9)/3\hbar \omega$ [which is the temperature where $\delta z_{\beta_{HT}} = 0.5$ for $z' = 0.8L_{TF}$; see Eq. 2]. Note that the true condensate is not to be confused with a BEC, and strictly only appears at zero temperature (Thomas-Fermi condensate; see 10). In the true condensate, the Green’s function and the momentum profile approach their temperature-independent ground state shapes, as shown by the convergence of $L_n/L_n^{sat}$ and $C(0,0.8L)$ in Fig. 4. The system becomes practically phase coherent, as illustrated in Fig. 3(d), where $\sqrt{n \rho_{ij}} \approx G(0,j)$. For the parameter set in Figs. 4, we find that $\beta_{TC} \approx 0.115(5)$ which agrees with the analytical estimate $\beta_{TC} = (U^2/6Nv_l^2)^{1/3} \ln(9)$ = 0.116.

We now study the appearance of a phase-fluctuating condensate depending on the system parameters $U$, $V_t$, and $N$. The WI limit is characterized by $\gamma = U/2n \ll 1$. We define the average density by $n = N/2L$. Since we find that $L$ equals $L_{TF}$ within error bars in all cases, we use $\gamma = (3U^4/4V_tN^2)^{1/3}$. Note that the magnitude of $\gamma$ in the inhomogeneous system differs from that in the homogeneous system. In Figs. 4(a)-4(c), we demonstrate the effect of varying the number of particles $N$ at on-site repulsion $U = 0.5$ and trapping $V_t = 0.01$. Both $\beta_{QC}$ and $\beta_{TC}$ decrease with increasing $N$, but since the change of $\beta_{QC}$ is much greater than that of $\beta_{TC}$, the region of the phase-fluctuating condensate, $s = \beta_{TC}/\beta_{QC}$, increases with increasing $N$. The effect of varying $U$ is illustrated in Figs. 4(d)-4(f), where $N = 2000$ and $V_t = 0.4$. Increasing $U$, causes $\beta_{QC}$ to decrease, while $\beta_{TC}$ increases. Thus $\beta_{TC}/\beta_{QC}$ grows with increasing $U$. More generally, the deeper we are in the Thomas-Fermi limit of large
fluctuating condensate is beautifully realized, however, the ground state, as can be seen in Fig. 5: the phase-hibits a qualitatively different behavior when approaching $\gamma$, the correlation hole in the central region of the condensate is larger. Clearly, the quantum depletion for the parameter sets in Fig. 3 is much more significant than for systems in the WI limit, since the number of particles with zero momentum $N(k = 0) = \sum_{j,j'} G(j,j')/M$ decreases if $G(j,j') < \sqrt{\mu \rho_j}$. We also observe this behavior if the density is smaller than 1 everywhere in the trap, and therefore exclude the possibility that it is an effect of the optical lattice. The shape of $G(0,j)$ is consistent with the two limiting cases, i.e. exponential decay in the strong-coupling limit, and phase-coherence [i.e. Eq.(2)] in the weak-coupling limit.

We conclude with a summary of our main results. In the mean-field, weakly interacting and Thomas-Fermi limits, both true a Thomas-Fermi condensate and a phase-fluctuating condensate emerge. Phase correlation properties, manifest in the characteristic decay of the single-particle density matrix, agree with surprising precision with the mean-field theory in [10]. In an intermediate-coupling regime, a true condensate no longer appears. The regime of the phase-fluctuating condensate persists even longer, extending to $T = 0$. We observe a qualitatively different decay of the Green’s function, which cannot be accounted for by mean-field studies.

We acknowledge helpful discussions with Y. Castin, G. Shlyapnikov and T. Esslinger. This work was supported by a CNRS PICS grant (G.G.B. and F.H.) and the Swiss National Science Foundation. The simulations were performed on the Hreidar Beowulf cluster at ETH Zurich.

$$\mu_T/\hbar \omega \sim [(NU)^4/V_t]^{1/6},$$ the larger is the size of the quasicondensate.

While for the parameter sets in Figs. 4(a)-4(e), good agreement of $G(0,j)$ with expression (2) is observed for all $\beta$, as well as $\beta_{TC} \approx \beta_T$, this does not apply to the example in Fig. 4(f), where $\gamma = 0.17$. Instead, $G(0,j)$ exhibits a qualitatively different behavior when approaching the ground state, as can be seen in Fig. 5, the phase-fluctuating condensate is beautifully realized, however, $G(0,j)$ does not approach $\sqrt{\mu \rho_j}$ for $T \to 0$, and cannot be described by Eq. (2).

We consider the effect of stronger interactions in the trapped system on the phase-correlation properties in more detail. In Fig. 6 we show the ground state profiles for $N = 300$, $V_t = 0.01$, $U = 2.0$ and $U = 5.0$, respectively. We observe the same qualitative behaviour of the saturated Green’s function as in Fig. 5. Close to the center of the cloud, where the density is higher, the decay of $G(0,j)$ is exponential; however, it broadens toward the outer, more diluted regions of the cloud. By comparing Figs. 6(a) and 6(b), it can be seen that for larger $\gamma$, the correlation hole in the central region of the condensate is larger. Clearly, the quantum depletion for the parameter sets in Fig. 6 is much more significant than for systems in the WI limit, since the number of particles with zero momentum $N(k = 0) = \sum_{j,j'} G(j,j')/M$ decreases if $G(j,j') < \sqrt{\mu \rho_j}$. We also observe this behavior if the density is smaller than 1 everywhere in the trap, and therefore exclude the possibility that it is an effect of the optical lattice. The shape of $G(0,j)$ is consistent with the two limiting cases, i.e. exponential decay in the strong-coupling limit, and phase-coherence [i.e. Eq.(2)] in the weak-coupling limit.

We conclude with a summary of our main results. In the mean-field, weakly interacting and Thomas-Fermi limits, both true a Thomas-Fermi condensate and a phase-fluctuating condensate emerge. Phase correlation properties, manifest in the characteristic decay of the single-particle density matrix, agree with surprising precision with the mean-field theory in [10]. In an intermediate-coupling regime, a true condensate no longer appears. The regime of the phase-fluctuating condensate persists even longer, extending to $T = 0$. We observe a qualitatively different decay of the Green’s function, which cannot be accounted for by mean-field studies.

We acknowledge helpful discussions with Y. Castin, G. Shlyapnikov and T. Esslinger. This work was supported by a CNRS PICS grant (G.G.B. and F.H.) and the Swiss National Science Foundation. The simulations were performed on the Hreidar Beowulf cluster at ETH Zurich.

References:
[1] N.D. Mermin and H. Wagner, Phys. Rev. Lett. 22, 1133 (1966).
[2] P.C. Hohenberg, Phys. Rev. 158, 282 (1967).
[3] L.P. Pitaevskii and S. Stringari, J. Low. Temp. Phys. 85, 377 (1991).
[4] J.W. Kane and L.P. Kadanoff, Phys. Rev. 155, 80 (1967); J. Math. Phys. 6, 1902 (1965).
[5] F.D.M. Haldane, Phys. Rev. Lett. 47, 1840 (1981).
[6] L. Reatto and G.V. Chester, Phys. Rev. 155, 88 (1967).
[7] M. Schwartz, Phys. Rev. B 15, 1399 (1977).
[8] W. Ketterle and N.J. van Druten, Phys. Rev. A 54, 656 (1996).
[9] D.S. Petrov, M. Holzmann, and G.V. Shlyapnikov, Phys. Rev. Lett. 84, 2551 (2000); D.S. Petrov, G.V. Shlyapnikov, and J.T.M. Walraven, ibid. 87, 050404 (2001).
[10] D.S. Petrov, G.V. Shlyapnikov, and J.T.M. Walraven, Phys. Rev. Lett. 85, 3745 (2000).
[11] I. Bouchoule, K.V. Kheruntsyan, and G.V. Shlyapnikov, Phys. Rev. A 75, 031606(R) (2007).
[12] C. Mora and Y. Castin, Phys. Rev. A 67, 053615 (2004).
[13] D.L. Luxat and A. Griffin, Phys. Rev. A 67, 043603 (2003).
[14] N.M. Bogoliubov, C. Malyshev, R.K. Bullough and J.
Timonen, Phys. Rev. A 69, 023619 (2004).

[15] Yu. Kagan, B.V. Svistunov, and G.V. Shlyapnikov, Sov. Phys. JETP 66, 480 (1987); Yu. Kagan, V.A. Kashurnikov, A.V. Krasavin, N.V. Prokof’ev, B.V. Svistunov, Phys. Rev. A 61, 043608 (2000).

[16] S. Dettmer et. al., Phys. Rev. Lett. 87, 160406 (2001); D. Hellweg et. al., Appl. Phys. B: Lasers Opt. 73, 781 (2001); S. Richard, F. Gerbier, J.H. Thywissen, M. Hugbart, P. Bouyer, and A. Aspect, *ibid.* 91, 010405 (2003); J. Esteve, J.B. Trebbia, T. Schumm, A. Aspect, C.I. Westbrook, and O. Bouchoule, *ibid.* 96, 130403 (2006); M. Hugbart et. al., Europ. Phys. Jour. D 35, 155 (2005).

[17] E.H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963); E.H. Lieb, Phys. Rev. 130, 1616 (1963).

[18] D. Jaksch, C. Bruder, J.I. Cirac, C.W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81 (1998) 3108.

[19] F. Dafolvo, S. Giorgini, L.P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71, 463 (1999).

[20] S.M.A. Rombouts, K. van Houcke, and L. Pollet, Phys. Rev. Lett. 96, 180603 (2006); K. van Houcke, S.M.A. Rombouts, and L. Pollet, Phys. Rev. E 73, 056703 (2006).