Quantum fluctuations and condensate fraction during time-of-flight expansion

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The quantum fluctuation effects in the time-of-flight (TOF) experiment for a condensate released from an optical-lattice potential is studied within the truncated Wigner approximation. By investigating both the spatial and momentum density distributions, we find that the condensate fraction decreases monotonically in time and hence cannot be measured in the standard TOF image. We then propose a semiquantitative analysis for such dynamical quantum-depletion process. Our study shows a universal algebraic decay of the true condensate fraction, and has a very good agreement with numerical results. We also discuss possible methods to determine the condensate fraction inside the optical lattice, and its implication to the TOF experiments in higher dimensional systems.

Experimental realization of the superfluid to Mott-insulator transition in ultracold bosonic atoms opens a new horizon of strongly correlated physics [1,2]. Among various kinds of experimental techniques, the time-of-flight (TOF) experiment is the most important tool to observe possible quantum orders and related correlations [3–5]. It is generally believed that the TOF image can be interpreted as the momentum distribution of the atom cloud, if (i) the final size of the atom cloud is much larger than the initial one and (ii) the interaction effect during the expansion is negligible. As a result, the sharp interference peaks near the zero and Bragg wave vectors can be interpreted as a signature of a Bose-Einstein condensation inside the optical lattice.

Recently, Gerbier *et al.* [6] showed that the condition (i) is usually not satisfied, because the required time scale is much larger than the feasible value in the present experiments. As for the condition (ii), it is argued that the interaction effects are negligible (or at most in the mean-field level) due to the sudden drop of the particle density [6–8]. Different from the condensate in a single trapping potential, however, particles loaded in an optical lattice contain a much stronger interaction energy (and hence quantum fluctuation). In principle, the interaction effect can be removed by using Feshbach resonance, but such a far-from-equilibrium quantum dynamical problem itself is still very interesting and worthy of further investigation. It may also provide valuable insights for studying other quantum orders through the TOF experiment.

In this Rapid Communication, we numerically and analytically investigate the quantum dynamics of the TOF experiment for an interacting condensate released from a one-dimensional (1D) optical-lattice potential. The quantum fluctuations are included within the truncated Wigner approximation (TWA). The common adapted empirical definition of the condensate fraction, measured from the bimodal fitting of a spatial distribution, is found to saturate at a value substantially smaller than the free expansion result. On the other hand, the true condensate fraction, which can be unambiguously determined in the momentum space at any moment, decreases monotonically in time due to the dynamical quantum depletion. We find that the decaying condensate fraction can be fitted very well by a simple algebraic function with a universal exponent, showing an interaction induced quantum decoherence effect. We also show the 2D results and find a similar quantum-depletion phenomenon. Our results provide a deeper understanding about such a far-from-equilibrium quantum dynamical process and can be applied to studying other quantum orders.

We consider ^{87}Rb atoms loaded in a 1D optical lattice with the scattering length, $a_s = 5.45$ nm, the lattice constant, $a = 0.5$ μm, and the lattice strength, $V_0 = 10$ E_R, where $E_R = 2\pi\hbar \times 2.3$ kHz is the recoil energy. The transverse confinement radius is $R = 0.11$ μm, the on-site interaction energy is $U = 0.2 E_R$. When $t > 0$, the lattice potential is turned off and atoms start to expand with the same transverse confinement (with an effective 1D interaction strength, $g_1 = \frac{4\pi\hbar^2 a_s}{2\pi R^2 m}$, where m is the atomic mass). We use three approximations for numerical studies: noninteracting expansion, Gross-Pitaevskii equation (GPE), and the truncated Wigner approximation (TWA), respectively. Note that the TWA can be shown to be *exact* in the short-time limit as well as in the weak interaction limit [9–11], and therefore is very appropriate for the study of TOF dynamics. In all of our following calculations, we apply the same initial condition, a pure condensate state with ten particles in ten lattice sites, for simplicity. Application of our results to different initial states (say Mott state or with finite thermal or quantum depletion) is feasible, but is not our interest in this Rapid Communication. Finally, we discretize the optical-lattice potential by eight minicells in space, and calculate the expansion dynamics of the whole system up to 2048 minicells. In other words, for the initial condensate of ten lattice sites, the atom cloud is allowed to expand at most 25 times larger than its initial size within $100 \, \hbar/E_R \sim 7$ ms.

In Fig. 1(a1)–(a4), we show the calculated spatial density distributions at different expansion times. We note that both the GPE (dotted red lines) and the TWA (solid blue lines) results show a strongly broadened central peak compared to the noninteracting result (dashed black lines), while the difference becomes much weaker in the two Bragg peaks. To
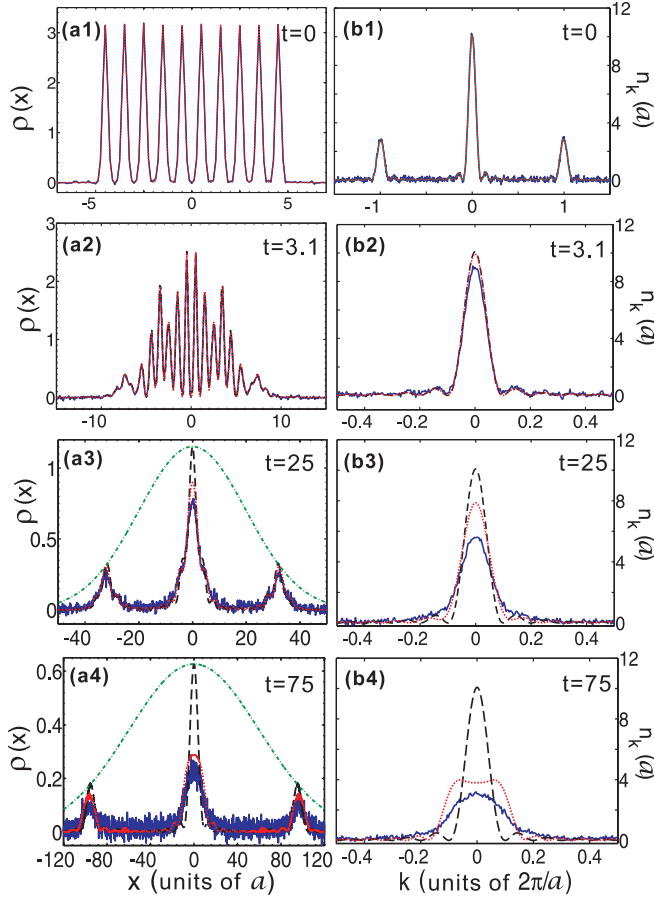
FIG. 1. (Color online) Time evolution of the spatial (a1)–(a4) and momentum (b1)–(b4) distributions for an interacting condensate released from a 1D optical lattice. The expansion time (t) is in the unit of $\hbar/E_R$. The dashed black, dotted red, and solid blue lines are the noninteracting, GPE, and TWA results, respectively. The dash-dotted green lines in (a3) and (a4) are proportional to the square of the expanding Wannier function. Other parameters are described in the text.

quantify such an interaction effect, we define the following renormalized peak ratio, η:

$$\eta(t) \equiv \frac{\rho(0,t)}{\rho(x(2\pi/a),t)} \frac{|\tilde{w}(2\pi/a)|^2}{|\tilde{w}(0)|^2}, \qquad (1)$$

where $\tilde{w}(k)$ is the Fourier transform of the Wannier function at the wave vector $k, x(k) = \hbar t k/m$, and $\rho(x,t)$ is the particle density at position x at time t. We note that η is exactly equal to one for a free expansion. This can be shown from the free expansion result: $\rho(x(\mathbf{k}),\mathbf{t}) \propto |\tilde{\mathbf{w}}(\mathbf{k})|^2 \mathcal{S}(\mathbf{k})$ [6], where the structure function, $\mathcal{S}(\mathbf{k})$, is a periodic function with the period $2\pi/a$, i.e., $\mathcal{S}(0) = \mathcal{S}(2\pi/a)$. Nevertheless, when the interaction is considered, our TWA result shows that η can be reduced to about 0.65 at $t = 75\hbar/E_R$ for the simulations in Fig. 1. In fact, similar experimental result has been observed in Ref. [12], where the population ratio of the first Bragg peak to the central peak is 35% larger than the ratio of a free expansion [i.e., $\eta(t) = \frac{1}{1.35} \sim 0.74$] at $t = 29.5$ ms. A systematic study on $\eta(t)$ should provide more information about the mean-field interaction effects during the TOF experiment.
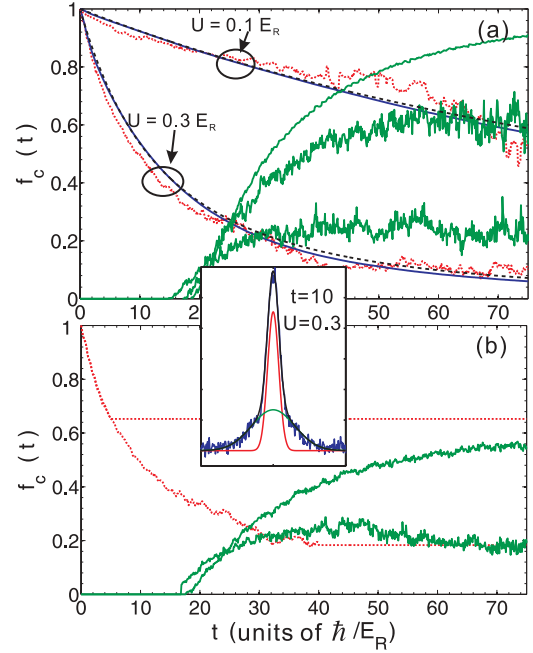

FIG. 2. (Color online) (a) Decay of the condensate fraction, $f_c(t)$ for different interaction energies, $U/E_R = 0.1$ and 0.3. The dotted red and solid blue lines are obtained from the bimodal fitting [13] in momentum distribution and wave function overlapping [14], respectively, while the dashed black line is fitted by Eq. (3). The three increasing green lines are the pseudocondensate fraction, $\tilde{f}_c(t)$, for $U/E_R = 0$, 0.1, and 0.3 (in the order from top to bottom). Inset is the momentum distribution with the bimodal fitting cures. (b) Same as the case in (a) for $U/E_R = 0.3$, but the interaction is turned off at $t_* = 5\hbar/E_R$ (upper line) and $t_* = 40\hbar/E_R$ (lower line), respectively.

At the first glance, the similar real space distributions of the GPE and TWA in Fig. 1(a1)–(a4) seem to suggest that the quantum fluctuation is negligible. However, from the momentum distribution shown in Fig. 1(b1)–(b4), one can see that the TWA result deviates from the noninteracting or the GPE results seriously: the condensate particles in the central peak are depleted and more noncondensate particles are generated with finite momenta, filling up the valleys of the initial momentum distribution. Note that the GPE result also has valleys after a longer time expansion, which simply results from the finite size effect of the initial wave function. In order to quantitatively investigate such a dynamical quantum depletion process, here we define the condensate fraction $f_c(t)$ to be the ratio between the number of condensate particles $N_c(t)$ near the zero momentum at time t to its initial value, i.e., $f_c(t) \equiv N_c(t)/N_c(0)$. We use two independent numerical methods to extract $f_c(t)$ from our TWA results: one is from the standard bimodal fitting of the central peak in the *momentum* distribution (see Ref. [13] and the inset of Fig. 2), and the other one is by calculating the probability to find particles in the condensate coherent state [14], which is supposed to follow the GPE result if no quantum fluctuation is included. In Fig. 2(a) we show the calculated results obtained from these two methods in the dotted red and solid blue lines, respectively, and find a very good agreement: the condensate fraction decreases monotonically during the TOF expansion and the

decay rate becomes larger for a stronger interaction. This quantum fluctuation effect cannot be obtained from our GPE (mean-field) results at all. We also note that when this method will fail automatically if the initial state is a normal or Mott state so that $N_c(0) = 0$.

For comparison, now we further calculate the pseudocondensate fraction, $\tilde{f}_c(t)$, which is extracted from the bimodal fitting in the *spatial* density distribution (see Ref. [13]), as the experimental convention. In Fig. 2(a), we show the calculated $\tilde{f}_c(t)$ (increasing green lines) for three different interaction strengths: it grows monotonically in time and eventually saturates at a value, $\tilde{f}_c(\infty)$, which is equal to one for a free expansion but smaller than one with a finite interaction. This result indicates that if the expansion is noninteracting, one can correctly measure the true condensate fraction after a long time expansion [$\tilde{f}_c(\infty) = 1$]. On the other hand, when the interaction is considered, $\tilde{f}_c(t)$ saturates at a value $\tilde{f}_c(\infty) < 1$, which cannot represent the true condensate fraction inside the optical lattice. Since the results shown in Fig. 2(a) are all calculated from the same initial condition, we conclude that the spatial density distribution (i.e., the TOF image) cannot give a good measurement of the condensate fraction during the TOF.

Although the time-dependence of the true condensate fraction, $f_c(t)$, and the pseudocondensate fraction, $\tilde{f}_c(t)$, are quite different, their close relationship can be revealed by switching off the particle interaction immediately at time t_* during the expansion. As shown in Fig. 2(b), $\tilde{f}_c(t)$ evolves eventually to a value set by the true condensate fraction at t_*, i.e., $\tilde{f}_c(\infty) = f_c(t_*)$, no matter its value is larger or smaller than $f_c(t_*)$. This is simply because, after t_*, particles expand freely in space and therefore the momentum distribution at t_* is transformed to the spatial distribution. This also confirms the decay of the condensate fraction. Note that, without turning off the interaction during the expansion, the true condensate fraction, $f_c(t)$, is hidden in the momentum distribution and therefore cannot be directly observed in the TOF image. However, turning off the interparticle interaction can also reduce the expansion speed, making it more difficult to reach the desired saturated value, $\tilde{f}_c(\infty)$.

The quantum depletion during the TOF can be viewed as a radiative process in the momentum space, where a pair of condensate particles are scattered out of the condensate and transfer their interaction energy toward the kinetic energy. Such dynamical process is governed by $H'_I = \frac{g_D}{2\Omega_D} \sum_{\mathbf{q} \neq 0} [b^\dagger_\mathbf{q} b^\dagger_{-\mathbf{q}} b_0 b_0 +$ H.c.], where g_D is the interaction strength in the D-dimensional free space, $b_\mathbf{q}$ is the boson operator, and Ω_D is the system volume. Here the scattering of particles in the Bragg peaks are neglected for simplicity. Denoting the many-body wave function at time t by $|\Psi_0(t)\rangle$, the many-body wave function at time $t + dt$ ($dt \to 0^+$) can be described by the following form: $|\Psi_0(t + dt)\rangle = B_0(dt)|\Psi_0(t)\rangle + \sum_\mathbf{q} B_\mathbf{q}(dt)|\Psi_\mathbf{q}(t)\rangle$, where $|\Psi_\mathbf{q}(t)\rangle \equiv N_c(t)^{-1} b^\dagger_\mathbf{q} b^\dagger_{-\mathbf{q}} b_0 b_0 |\Psi_0(t)\rangle$ and $B_\mathbf{q}(dt)$ is the associate coefficient. The noncondensate particle number, $\langle \Psi_0 | b^\dagger_\mathbf{q} b_\mathbf{q} | \Psi_0 \rangle$, has been neglected when compared to $N_c(t) \equiv \langle \Psi_0(t) | b^\dagger_0 b_0 | \Psi_0(t) \rangle$ in the normalization constant. Therefore, the condensate particle number at $t + dt$ becomes $N_c(t + dt) = N_c(t) - 2 \sum_\mathbf{q} |B_\mathbf{q}(dt)|^2$. Giving $B_i(0) = \delta_{i,0}$, we can apply the spirit of Fermi-Golden rule for

$dt \to 0$, and obtain the decay rate of the condensate density $n_c(t) \equiv N_c(t)/\Omega_D$ by

$$\frac{dn_c}{dt} = -\frac{4\pi}{\hbar} \frac{1}{\Omega_D} \sum_{\mathbf{q} \neq 0} |\langle \Psi_\mathbf{q} | H'_I | \Psi_0 \rangle|^2 \delta(2\mu_D - \hbar^2 \mathbf{q}^2/m),$$

$$\approx -\frac{4\pi}{\hbar} \frac{2g_D^2 N_c(t)^2}{2\Omega^2} \int \frac{d^D\mathbf{q}}{(2\pi)^D} \delta(2\mu_D - \hbar^2 \mathbf{q}^2/m),$$

$$\approx -\frac{2C_D}{D} g_D^2 n_c(t)^2 \mu_D^{D/2-1}, \tag{2}$$

where $C_D \propto \frac{1}{\hbar}(\frac{m}{\hbar^2})^{D/2}$ is a constant, and μ_D is the chemical potential in the D-dimensional space. We note that in general μ_D depends on the interaction strength, global trapping potential, dimensionality, etc. For example, in a uniform 3D system, $\mu \sim g_3 n_c$ in the weakly interacting limit, while there is no condensate particles in a uniform 1D system. For a 1D finite size interacting system here, without loss of generality, we may simply assume $\mu_D = \epsilon_D n_c$, where ϵ_D should depend on the interaction strength as well as system size. After integrating over this differential equation, we obtain the condensate fraction, $f_c(t) \equiv n_c(t)/n_c(0)$, as follows:

$$f_c(t) = \left[\frac{1}{1 + \tilde{C}_D n_c(0)^{D/2} g^2 t} \right]^{2/D}, \tag{3}$$

with a nonuniversal fitting parameter here $\tilde{C}_D \equiv C_D \epsilon_0^{D/2-1}$ (depending on finite size effect, finite temperature, initial noncondensate particles, etc.). It is important to note that, instead of an exponential decay expected in a regular radiative process, the many-body interaction matrix element, H'_I, couples the decay rate to the condensate density, so that it becomes an algebraic decay instead. If the initial state is not a pure condensate, Eq. (3) should be still valid if only away from the regime of quantum phase transition or Mott phase. Using Eq. (3) to fit our TWA results shown in Fig. 2(a) with a fitting parameter $\tilde{C}_D$, we find a very good agreement to confirm the quantum fluctuation effects on the condensate fraction during the TOF experiment.

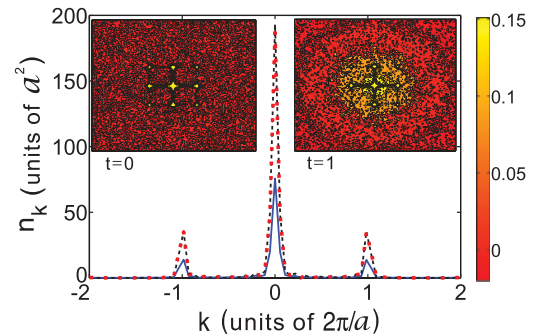As for higher dimensions, in Fig. 3, we also show the momentum distribution of atom clouds expanding in a

FIG. 3. (Color online) Momentum distribution of a TOF expansion in 2D space along $y = 0$ at $t = \hbar/E_R$. The dashed black, dotted red, and solid blue lines are the noninteracting, GPE, and TWA results, respectively. (The first two cannot be distinguished here.) The two insets show the momentum distributions for TWA at $t = 0$ and $t = \hbar/E_R$, respectively. Here the interaction energy is larger ($U = 0.45E_R$) in order to demonstrate the quantum depletion effects within a short time expansion.

2D system from an initial 11×11 lattice sites (total 128×128 minicells). Due to the limitation of our computational resources, only results of a very short time expansion can be obtained before atoms reach the boundary. No quantitative information can be extracted yet. However, by comparing the momentum distributions in the GPE and TWA results, it is easy to find the decay of condensate density even in such a short-time regime due to the quantum fluctuations.

Before concluding, we mark several aspects to discuss: (i) We have also calculated the TOF dynamics of 20 atoms in ten lattice sites (not shown here), and find a stronger decay of $f_c(t)$ for the same interaction strength. However, results of 20 particles in 20 wells are found almost the same as results of ten particles in ten wells. This shows that the system size is not relevant here, and its dependence of the particle density (rather than total particle number) is also consistent with the nature of quantum fluctuations. (ii) Since TOF is known as a far-from-equilibrium dynamical process, the integrability of 1D Bose gas should be irrelevant to any of our results here. This is also confirmed by the similar depletion process in

2D systems shown in Fig. 3. (iii) From Eq. (3), it is easy to see that for an expansion in higher dimensional systems, the exponent of decay becomes smaller, due to the smaller density of states in the long-wavelength limit. This is therefore also consistent with the general principle that the quantum fluctuation effects become smaller in higher dimensional systems.

In conclusion, we numerically and analytically study the interaction effects for an expanding condensate released from an optical lattice. The condensate fraction has an algebraic decay in time due to the quantum fluctuation effects. Our results provide a deeper understanding to the quantum fluctuation effects during the time-of-flight experiment.

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[13] Our bimodal fitting process is as follows: We first set a reasonable momentum k_0 and fit the distribution by a Gaussian function for $|k| > k_0$. After subtracting this first fitting curve, we fit the residual distribution by a second Gaussian function for $|k| < k_0$. The area of the second fitting result gives $N_c(t)$, which is checked to be independent of k_0. Condensate particles at Bragg peaks are neglected. Similar method is applied to extract $\tilde{f}_c(t)$ from the real space distribution.

[14] The condensate density obtained from the wave fuction overlapping method is to calculate $\langle \hat{b}_{GP}^+(t)\hat{b}_{GP}(t)\rangle$, where $\hat{b}_{GP}(t) \equiv \int \psi_{GP}^*(x,t)\hat{\psi}(x)\,dx$ is the operator projected onto a Gross-Pitaevskii state, $\psi_{GP}(x,t)$. Here $\hat{\psi}(x)$ is the field operator. See also M. J. Steel *et al.*, Phys. Rev. A **58**, 4824 (1998).