Condensate Fraction in a 2D Bose Gas Measured across the Mott-Insulator Transition

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We realize a single-band 2D Bose-Hubbard system with Rb atoms in an optical lattice and measure the condensate fraction as a function of lattice depth, crossing from the superfluid to the Mott-insulating phase. We quantitatively identify the location of the superfluid to normal transition by observing when the condensed fraction vanishes. Our measurement agrees with recent quantum Monte Carlo calculations for a finite-sized 2D system to within experimental uncertainty.

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Measurements of condensed matter systems realized by cold atoms in optical lattices are now performed with sufficient accuracy to compare with *ab initio* calculations [1–3]. Bosonic atoms in a lattice nearly perfectly realize the iconic Bose-Hubbard (BH) Hamiltonian. Here, we study the system's momentum distribution, measure the condensate fraction, and accurately identify the transition point from the low temperature superfluid (SF) phase by identifying when the condensate fraction vanishes.

The SF to Mott-insulator (MI) transition can be accessed by changing the depth of the optical potential [4], and has been observed in 1D, 2D, and 3D [2,5,6]. A range of studies have verified the understanding of the MI phase in 2D and 3D [1,2,7,8]. In contrast, the SF phase and the details of the transition to MI have gone largely unstudied. The only quantitative measurement locating the transition is in 3D and is not in agreement with theory [3]. We focus specifically on the superfluid phase of a 2D system and its transition to a normal state: we observe the expected increasing momentum spread and vanishing condensate fraction as the system leaves the SF phase. The transition point agrees with the best available calculations [9], thereby locating a point on the nonzero temperature 2D BH phase diagram. The condensate fraction in our nonzero temperature system vanishes more sharply than expected for a zero temperature inhomogenous system, confirming that the superfluid regions are rapidly driven normal when an insulator appears [10,11].

The physics of interacting systems frequently depends on dimensionality: in 3D the SF is a conventional Bose-Einstein condensate (BEC); in 2D, a Berezinskii-Kosterlitz-Thouless (BKT) SF; finally, in 1D there is no true SF. In contrast, only the detailed properties of the MI phase depend on dimensionality. In the $T > 0$, 2D case studied here, the existence of Bose condensation is a consequence of the finite size of our trapped system. We associate bimodal momentum distributions with the SF phase, and use fits to the distribution to identify the Bose-condensed fraction and thereby measure the transition point between SF and normal.

At low temperature the transition from SF is to a normal state which crosses over to MI as the lattice depth increases [10,11]. As a result any $T > 0$ measurement based on condensate fraction will identify the SF to normal transition but will be largely insensitive to the subsequent crossover to MI.

We study samples of rubidium atoms in a sinusoidal plus harmonic potential. For atom occupancy per lattice site larger than unity [6,12], the low temperature SF phase (shallow lattice) is expected to evolve into a structure composed of alternating shells of SF and MI (deep lattice). As the lattice deepens, each successive MI region appears and grows, as probed in Ref. [8]. At $T = 0$ the amount of SF varies smoothly with lattice depth giving no abrupt changes in the momentum distribution to indicate a phase transition. In this Letter, we simplify the situation by working near unit filling, where the only insulating phase is unit-occupied MI; thus, any observed signature can only be the transition from SF to normal. Recent experiments have shown that weak interactions lead to a decrease in the 2D BEC transition temperature [13]. Lattice potentials increase the relative importance of interactions; indeed, the onset of the MI phase corresponds to driving the critical temperature to zero.

The BH model describes lattice bosons with a hopping matrix element t, and an on-site interaction energy U. The physics of the BH model depends only on U/t [14]. In an infinite, homogenous $T = 0$ 2D system, the transition from SF to MI occurs at $(U/t)_c \approx 16.5$ [9,15–17]. Remarkably, we observe a sharp transition at $U/t = 15.8(20)$ [18] in our $T > 0$, finite-sized, harmonically trapped system.

Our data consist of images of atom density after sudden release and time-of-flight (TOF), approximating the *in situ* momentum distribution. Figure 1 shows 2D momentum distributions (right) and cross sections (left). As evidenced by Figs. 1(a) and 1(b) each diffraction order in the momentum distributions consists of a narrow peak on a broad pedestal. Fitting to a bimodal distribution (see below), we determine f, the fractional contribution of the narrow component, and identify f as the "condensate" fraction.

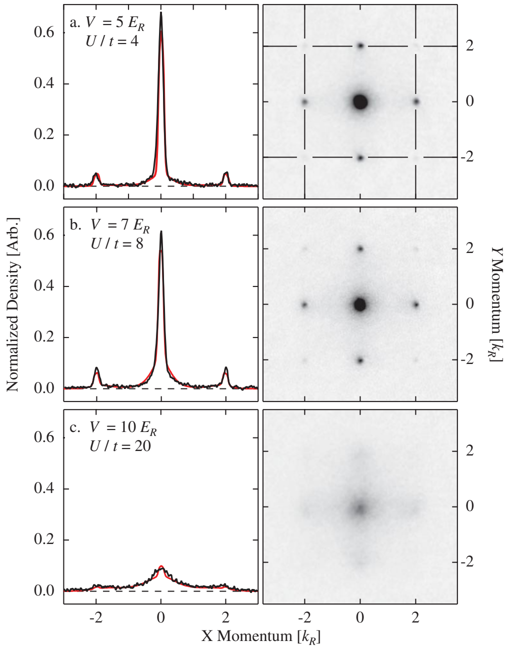

FIG. 1 (color). Momentum distributions and cross sections at $U/t = 4(1)$, 8(1), and 20(2). Each row shows a single momentum distribution normalized by the total atom number; the lines in the top right panel indicate trajectories along which four cross sections were taken. The left panel shows the average of these four sections (black solid line); the red dashed lines denote the fit to the bimodal distribution.

We associate images with non-negligible f as being in the SF phase [19]. We emphasize that superfluidity is a transport phenomena and cannot unambiguously be associated with features in the momentum distribution [10,11,20]. This association is also imperfect at $T > 0$ because in 2D trapped systems we expect a discernible condensate fraction even after the vortex pairs of a BKT SF unbind [21], destroying the 2D SF. f vanishes only when the resulting phase-fluctuating quasicondensate vanishes [13,22].

To characterize the transition from SF to normal, we extract two independent quantities from TOF images: f, and an "energy scale" σ. We also measure a related quantity, the full width at half maximum (FWHM) Γ of the quasimomentum distribution, which we compare to theory. As the lattice depth is increased f vanishes concurrently with a sudden increase in Γ, abrupt signatures that we associate with the transition.

We produce nearly pure 3D ^{87}Rb BECs with $N_T = 1.2(4) \times 10^5$ atoms in the $|F = 1, m_F = -1\rangle$ state [2]. A pair of linearly polarized, $\lambda = 820$ nm laser beams forms a $30(2)E_R$ deep vertical optical lattice along $\hat{z}$ that divides the 3D BEC into about 70 2D systems (turn-on time = 200 ms). The single photon recoil wave vector and energy are $k_R = 2\pi/\lambda$ and $E_R = \hbar^2 k_R^2/2m = h \times 3.4$ kHz; m is the atomic mass and h is Planck's constant. The largest 2D system, containing ≈ 3000 atoms, has a chemical potential $\mu_{2D} = h \times 600(100)$ Hz and we measure a temperature $k_B T = k_B \times 33(4)$ nK $= h \times 700(70)$ Hz. Since the first vibrational spacing $h \times 33(1)$ kHz $\gg \mu_{2D}, k_B T$, this system is well into the 2D regime. In addition, a weaker, square 2D lattice in the $\hat{x}$-$\hat{y}$ plane is produced by a second beam arranged in a folded-retroreflected configuration [23], linearly polarized in the $\hat{x}$-$\hat{y}$ plane (turn-on time = 100 ms [24]). The intensities of both lattices follow exponentially increasing ramps, with 50 and 25 ms time constants, respectively, and reach their peak values concurrently. These time scales are chosen to be adiabatic with respect to mean-field interactions, vibrational excitations, and tunneling within each 2D system. The final depth of the $\hat{x}$-$\hat{y}$ lattice determines U/t and ranges from $V = 0$ to $25(2)E_R$ [25]. The lattice depths are calibrated by pulsing the lattice for 3 μs and observing the resulting atom diffraction [26].

We calculate U/t using a 2D band-stucture model and the s-wave scattering length [27]. The $\pm 10\%$ uncertainty in U/t stems from the uncertainty in lattice depth [28].

Once both lattices are at their final intensity, the system consists of an array of 2D gases each in a square lattice of depth V with a typical density of 1 atom per lattice site. The atoms are held for 30 ms, and all confining potentials are abruptly removed (the lattice and magnetic potentials turn off in $\lesssim 1$ μs and $\simeq 300$ μs, respectively). Initially confined states are projected onto free particle states which expand for a 20.1 ms TOF [29], when they are detected by resonant absorption imaging. Apart from effects of atomic interactions during expansion and the initial size of the sample, initial momentum maps into final position, so each image approximates the $\hat{x}$-$\hat{y}$ projection of the momentum distribution. We fit each momentum distribution to a simple function which describes the distributions over the full range of U/t studied here, with just three free parameters.

First, we model the broad background as a thermal distribution of noninteracting classical particles in a 2D sinusoidal band with states labeled by quasimomentum q_x and q_y, $n(q_x, q_y) \propto \exp[2(\cos\pi q_x/k_R + \cos\pi q_x/k_R)/\sigma]$; this contributes two fitting parameters: σ and the noncondensed atom number. In the shallow lattice limit, σ gives the temperature, $\sigma = k_B T/t$. This fit does not distinguish atoms thermally occupying higher momentum states from atoms occupying these states in the ground state wave function, i.e., from the quantum depletion of the SF. $n(q_x, q_y)$ multiplied by a suitable Wannier function correctly describes the momentum distribution of atoms in the MI phase to first order in t/U where $\sigma = U/4t$ is unconnected to temperature. Our function fits the random phase approximation (RPA) momentum distribution fairly well even as higher order terms become important [2,30].

The second portion of the momentum distribution consists of a narrow peak, which we interpret as Bose-condensed atoms. We take the narrow peak to be the inverted parabola of a Thomas-Fermi profile (of fixed width for all comparable data [31]), characterized by a single fitting parameter, condensed number.

The observed condensate peak width after TOF stems largely from initial system size, not interaction effects during TOF or the initial momentum spread. Here interactions during TOF are reduced due to rapid expansion along $\hat{z}$ after release from the tightly confining vertical lattice. Our analysis further reduces these interaction effects by excluding data inside the first Brillouin zone, with the highest density. This decreases the measured FWHM of the peak from 30(1) to 22(1) μm (from $0.26k_R$ to $0.21k_R$). Changing the TOF from 20.1 to 29.1 ms only increased the FWHM from 22(1) to 28(1) μm (from $0.21k_R$ to $0.17k_R$).

Figure 2(a) shows that as V increases, f vanishes at a critical value $V_{\rm crit}$, while the total atom number remains constant. We verified this disappearance does not result from excessive irreversible heating of the system by exceeding $V_{\rm crit}$, then lowering the lattice and observing a condensed fraction [6].

To gain a *qualitative* understanding of the vanishing condensate fraction, we performed a nonzero temperature mean-field theory (MFT) simulation of an array of 2D BH systems in a 3D harmonic trap [32]. At $T > 0$ we determine the entropy at small U/t that gives the observed $\approx 45\%$ condensate fraction, and assume this entropy is unchanged as V increases. The red dashed line in Fig. 2(a) shows the MFT condensate fraction vs V at constant entropy. Given that $T = 0$ MFT overestimates the transition [$(U/t)_{\rm MFT} =$ 23.3, compared to $(U/t)_c = 16.5$ from more accurate calculations], the curve unexpectedly lies on the data. MFT also gives f as function of U/t in units of $(U/t)_c$. We identify the transition point by fitting this function to the data allowing $(U/t)_c$ to vary, yielding $(U/t)_c = 15.8(20)$ [a lattice depth $V_{\rm crit} = 9.0(5)E_R$].

Figure 2(b) displays σ from the uncondensed background portion of the distribution. At large V we recover the behavior expected in the MI phase; this measurement is equivalent to observations of the modulated momentum distribution in the MI phase [1,2]. σ is monotonic with V, varying smoothly across $V_{\rm crit}$. This is in agreement with RPA theory where the onset of superfluidity affects only states near zero quasimomentum. Figure 2(b) shows that when $V \lesssim 4E_R$ ($U/t \lesssim 3$), $k_BT/t \approx 2.0(3)$. Extrapolating to $V = 0$ gives $k_BT = E_R\sigma/\pi^2 \approx k_B \times 33$ nK (valid when $T \ll E_R$). This temperature is well below the $k_B \times$ 45 nK expected for noninteracting particles in our 2D harmonic trap with $f = 0.45$; this reduction is similar to that observed in Ref. [13], which focused on 2D atomic systems with no 2D lattice.

A related characterization of the system is the FWHM Γ of the quasimomentum distribution [6,9,17,19,33]. Figure 3 shows the width of the 2D distributions (see Ref. [2]) as a function of V. In the SF phase Γ hardly depends on V since the dominant feature of the distribution is the condensate peak. Γ only begins to change very close to the SF to normal phase transition when the heights of the components of the bimodal distribution become comparable (when the condensate disappears), consistent with calculations in homogenous and trapped systems [9]. We calculate Γ in the MI phase in the RPA [30] which accurately connects to the large U/t limit ($\sqrt{2}k_R$ along $\hat{x} + \hat{y}$ and k_R along $\hat{x}$). In the RPA, Γ is a function of U/t in units of $(U/t)_c$. The red dashed lines are fits to the measured widths using two free parameters (joint between both panels): in the MI region we use the RPA functional form with $(U/t)_c$ as the first fit parameter, and the constant width in the SF phase is the second. We obtain $(U/t)_c =$ 16.7(20), in accord with the $(U/t)_c = 15.8(20)$ from our fit to the condensate fraction.

We identify the point when the condensate fraction vanishes (and Γ abruptly increases) with the onset of the SF to normal transition, i.e., when a normal region begins to rapidly expand in our inhomogeneous system. (Our measured visibility, computed as in Refs. [1,7], abruptly drops from near unity at $U/t \approx 16$.) Accurate numerical calculations give values of $(U/t)_c$: 16.25(10) [9] and 16.77 [17]. Perhaps most relevant are quantum Monte Carlo (QMC) calculations which include the effects of harmonic confinement; in this case, Wessel *et al.* [9] find that a MI region first forms at $(U/t)_c = 17.2$ [the exact value of $(U/t)_c$ depends on the details of the harmonic potential]. Both values lie within our experimental uncertainty.

The calculations [9,17] are at zero temperature, and while they agree with our observed $(U/t)_c$, they do not

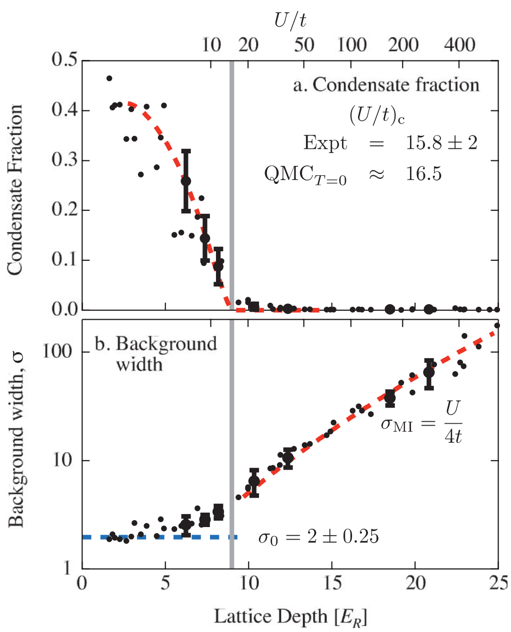

FIG. 2 (color). Condensed fraction f and σ vs V (bottom axis) or U/t (top axis). The dots denote values determined from 2D fits to the full momentum distribution: small dots result from one image and the large dots indicate data averaged over about 20 separate images. The uncertainties are their root mean squared variation, and are indicative of the single-image uncertainties. (a) Condensate fraction. The red dashed line is computed from our MFT model. (b) Fit parameter σ. At low U/t σ is nearly constant (blue dashed line), from which we infer an initial temperature $k_BT \approx 2t$. At large U/t σ monotonically increases, consistent with predictions of perturbation theory in the MI phase (red dashed line).

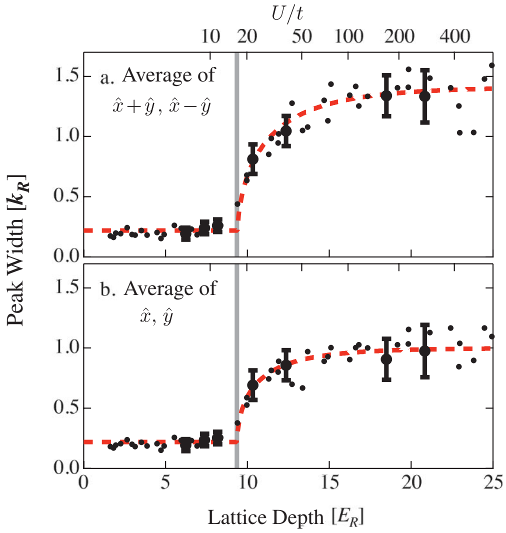

FIG. 3 (color). Quasimomentum width vs V (bottom axis) or U/t (top axis). The symbols denote the average FWHM of the quasimomentum distribution along the axes of highest symmetry (top: averaged along $\hat{x}+\hat{y}$ and $\hat{x}$-$\hat{y}$; bottom: averaged along $\hat{x}$ and $\hat{y}$). The small and large dots and uncertainties are as explained at Fig. 2. The red dashed line is the horizontally displaced RPA momentum width, as discussed in the text, and the vertical gray line denotes the location of the SF-normal transition identified from the sudden increase in Γ.

predict a sudden increase in peak width or a vanishing condensate fraction at $(U/t)_c$. At $T = 0$ and as U/t increases past $(U/t)_c$, where an inhomogeneous system first develops a unit-occupied Mott core, the shell of SF persists to large U/t. Thus, at $T = 0$, f drops rapidly at $(U/t)_c$, but does not vanish. Our system, however, is at $T > 0$, with a reduced condensate fraction of $\approx 45\%$ for small V. Our MFT model shows that this temperature quickly drives the SF shells to the normal phase as U/t increases past $(U/t)_c$. As a result the SF shells rapidly go normal, and then Mott regions form (see Refs. [10,11,34]). That this feature is seen in preliminary $T > 0$ QMC calculations [33] underscores the need for further $T > 0$ calculations to compare with experiment.

This experiment constitutes the measurement of a single point of the nonzero temperature 2D BH phase diagram. We expect future experiments will expand on this result at different temperatures, densities, in different dimensions, and in traps with more homogenous density distributions; new theory should aid in the interpretation of these experiments.

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