Single-atom-resolved probing of lattice gases in momentum space

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Measuring the full distribution of individual particles is of fundamental importance to characterize many-body quantum systems through correlation functions at any order. Here we demonstrate the possibility to reconstruct the momentum-space distribution of three-dimensional interacting lattice gases atom-by-atom. This is achieved by detecting individual metastable Helium atoms in the far-field regime of expansion, when released from an optical lattice. We benchmark our technique with Quantum Monte-Carlo calculations, demonstrating the ability to resolve momentum distributions of superfluids occupying 10^5 lattice sites. It permits a direct measure of the condensed fraction across phase transitions, as we illustrate on the superfluid-to-normal transition. Our single-atom-resolved approach opens a new route to investigate interacting lattice gases through momentum correlations.

Ultracold atoms in optical lattices have proven to be a valuable system to investigate condensed-matter models in a tunable and controllable environment [1]. In this context, the past decade has witnessed the emergence of a new generation of lattice experiments capable of measuring spatial distributions and correlations between individual particles [2–8]. These apparatus have paved the way to unprecedented investigations of both equilibrium and dynamical properties of strongly-interacting matter. Similarly, the on-site detection of individual spins is central to other experimental platforms, like trapped ions [9] or superconducting circuits [10]. Some paradigmatic manifestations of quantum many-body effects are however elusive in spatial correlations, and multi-particle correlations between other degrees of freedom play a fundamental role [11].

In this respect, the momentum of the particles is an essential degree of freedom, whose correlation functions contain unique signatures of many-body quantum coherence. Off-diagonal long-range order and Bose-Einstein condensation manifest in the momentum density [12], and thermal and quantum fluctuations can be characterized through the population of one-particle momentum states [13]. While well established for weakly-interacting gases, these properties are notoriously difficult to measure in strongly interacting systems like liquid Helium [12]. Two-particle momentum correlations are central to various microscopic mechanisms of pairing in many-body Hamiltonians, from the quantum depletion in Bose liquids to fermionic Cooper pairing [12], and they exhibit signatures of quantum phase transitions [14] and out-of-equilibrium dynamics [15]. Creating the possibility to measure the momentum distribution of individual particles would permit a direct assessment of these many-body phenomena.

In principle, quantum gases offer the possibility to explore the momentum degree of freedom by performing time-of-flight (TOF) experiments, i.e. probing the gas after a free-fall expansion. In practice, the conditions under which the measured distributions precisely map to the in-trap momentum distributions are difficult to fulfill [16]. The free-fall dynamics should not be perturbed by the presence of interactions, a situation that can be achieved when atoms are released from an optical lattice without tuning the interaction strength to zero [17, 18]. In addition, a sufficiently long TOF is required to enter the far-field regime of expansion, well beyond those implemented so far [17]. Such a long TOF implies probing extremely dilute clouds over a large volume, a situation for which optical probes are not adapted. Moreover the technical requirements to efficiently collect the photons emitted by a single atom make it difficult extending single-atom fluorescence techniques to the far-field.

In this Letter, we demonstrate the ability to reconstruct, accurately and atom-by-atom, the three-dimensional momentum distribution of strongly-interacting lattice gases. We benchmark our apparatus with ab-initio Quantum Monte-Carlo (QMC) calculations in the Bose-Hubbard regime. Accessing the momentum distributions of interacting lattice gases allows us to introduce a thermometry method from the comparison with QMC calculations and to directly measure the condensed fraction f_c. Finally, we monitor f_c across the superfluid-to-normal phase transition, illustrating the capabilities offered by our apparatus.

Our approach exploits the properties of Helium-4 atoms brought to quantum degeneracy in a metastable state (^4He*). On the one hand, the large internal energy of ^4He* yields the unique possibility to detect individual atoms in three dimensions over centimeter distances [19], in contrast to optical imaging methods. On the other hand, the original combination of a long time-of-flight t_TOF = 325 ms and the small mass of ^4He* allows us to probe the far-field. Entering the far-field regime necessitates a TOF larger than t_{pol} ≃ mL^2/2\hbar [17], where \hbar is the reduced Planck constant, m the atomic mass and L the length of the trapped gas. The use of a light atomic species is thus extremely favorable to keep t_{pol} accessible, even for large system sizes L. For our parameters (L ~ 50 lattice sites), we find t_{pol} ≃ 50 ms, indeed much
We realize strongly interacting lattice superfluids by adiabatically loading a Bose-Einstein Condensate (BEC) of $N = 40(4) \times 10^5$ $^4$He* atoms [21] in the lowest energy band of a cubic optical lattice. The lattice spacing is $a = 775 \text{ nm}$ and its amplitude $V_L = 9.6(3) E_R$ is fixed, where $E_R = \hbar^2/8ma^2$ is the recoil energy. At this amplitude $V_L$, we have $U/J = 9.5$, where $U$ and $J$ are the Bose-Hubbard on-site interaction and tunneling energy parameters, and the expected quantum depletion is large ($\sim 15\%$), highlighting the presence of strong quantum correlations. After abruptly switching off the optical lattice, the cloud expands for $t_{\text{TOF}} = 325 \text{ ms}$ and it is probed with the Helium detector (Fig. 1(a)). The Helium detector yields 3D distributions of individual atoms as shown in Fig. 1(b) and has been described previously [13, 22]. In brief, metastable atoms hit the surface of a pair of micro-channel plates (MCPs) from which they can extract an electron by releasing their internal energy (19.6 eV). The pair of MCPs multiplies the electron emitted by a single $^4$He* atom and, in combination with a delay-line anode, allows to reconstruct the 3D position $\vec{r}$ of the atom in the frame of the cloud center-of-mass [13], with a detection efficiency of 25(5)%. To relate the position $\vec{r}$ of an atom to the in-trap momentum $\hbar \vec{k}$, we use the ballistic formula $\hbar \vec{k} = m \vec{r}/t_{\text{TOF}}$. This relation is expected to be accurate when atoms are released from a lattice of moderate amplitude at low filling [17, 18]. Our experiment is performed under these conditions and we do not observe modification of the TOF distribution induced by interactions (see below).

We now turn to the benchmarking of the measured atom distributions. Our experiment simulates the Bose-Hubbard Hamiltonian (BHH) that is numerically solvable using Quantum Monte-Carlo (QMC) approaches [23]. We thus compare experimental data with ab-initio QMC calculations of the in-trap momentum distribution $n(\vec{k})$. (a) Log-plot of 1D cuts $n(k,0,0)$ through the measured 3D distribution $n(\vec{k})$ (orange), and through the QMC momentum distribution (dashed line) obtained for our experimental parameters and $T = 3.9 \text{ J}$. The temperature $T$ is the only adjustable parameter (see text). The measured amplitude of the central peak is slightly affected by a saturation of the Helium detector (see text). (b) 1D cuts $\tilde{n}(k,0,\pm k_a)$ compared to the QMC profile $n(k,0,0)$. The height of the central peak of these distributions has been normalized to one. Saturation effects are not present on the first- and second-order peaks of diffraction.
In a box centered at $\vec{k} = (k, 0, 0)$ of size $(\Delta k, 3\Delta k, 3\Delta k)$ with $\Delta k = k\alpha/160$ where $k\alpha = 2\pi/a$. The QMC calculations are performed with the experimental parameters, except for the temperature – not measured in the experiment – which is the only adjustable parameter [20]. To take into account the efficiency of the detection process, we rescale the experimental data by that of the condensate manifesting as sharp peaks on top of the broad distribution of depleted atoms $n_{\text{NC}}(\vec{k})$ (both quantum and thermal depletion),

$$n(\vec{k}) = n_0(\vec{k}) + n_{\text{NC}}(\vec{k}).$$

The condensate has long-range phase coherence and $n_0(\vec{k})$ has a Fourier-limited width $\propto 1/L$. On the other hand, $n_{\text{NC}}(\vec{k})$ is a smoothly varying distribution with a typical momentum width $\propto 1/\alpha$ given by the lattice density of state. This results from the population of all quasi-momentum states by the quantum depletion at $U/J = 9.5$ and by the thermal depletion at non-vanishing temperatures. For large trapped systems, $L \gg \alpha$, $n_0$ and $n_{\text{NC}}$ thus clearly separate in the momentum space with the condensate manifesting as sharp peaks on top of the broad distribution of depleted atoms [25]. In the following we exploit this separation of scales to calibrate the temperature and measure the condensed fraction.

To determine the temperature, we use the com-
comparison with QMC, inspired by the pioneering work of [26]. Here we measure a single parameter \( r_T = n(k_0, 0, 0)/n(k_0/2, 0, 0) \) to be matched with QMC numerics. The variation of \( r_T \) with \( T \) obtained from the QMC calculations is shown in Fig. 3. In the regime of the experiment, \( r_T \) varies by 4 orders of magnitude when \( T \) increases only by a factor 3, yielding an unprecedented precision in the calibration of the temperature. Using a controlled heating sequence, we have varied the temperature in the experiment at a fixed \( U/J = 9.5 \) [20]. By comparing the measured \( r_T \) with the thermometry curve we obtain \( T \) with a 5% uncertainty, limited by the experimental uncertainty on the atom number. In Fig. 3 we also show comparisons of the measured 1D cuts \( n(k, 0, 0) \) with QMC calculations performed at the temperature obtained from the measurement of \( r_T \). The excellent agreement over the entire range of temperatures validates the thermometry method. The thermometry curve in Fig. 3 applies to the BHH (with our parameters) and is model-dependent. But the central idea of the method – probing low-energy excitations, the population of which strongly varies with the temperature – can be generalized to a large variety of Hamiltonians.

The condensed fraction \( f_c \) is a central quantity to investigate finite-temperature phase diagrams [27]. But measuring \( f_c \) in many-body systems is challenging as the strong interactions make it difficult to probe single-particle states and access \( n(\vec{k}) \). Techniques like neutron scattering in liquid Helium indeed fail to separate the condensate from the depleted atoms [12] while Bragg spectroscopy in strongly interacting gases necessitates switching off the interactions [28]. Overcoming the difficulties associated to accessing \( n(\vec{k}) \) [16, 29], our apparatus provides the first direct measurement of \( f_c \) in a 3D lattice experiment. We identify the momentum \( k_0 \) where the contributions of \( n_0 \) and \( n_{NC} \) separate on the 1D profiles [20]. We then use the full 3D distribution to count the fraction \( f_c \) of atoms of the first Brillouin zone contained in a sphere of radius \( k_0 \) centered on \( \vec{k} = 0 \). We plot \( f_c \) as a function of \( T \) in Fig. 4. In the absence of a theoretical model, we extract the critical temperature using an empirical function [29], obtaining \( T_c = 5.9(2) J \). Our approach allows us to observe the onset of BEC in a deep lattice with unprecedented resolution.

An interesting question is whether a trapped gas can provide information about the phase diagram of homogeneous systems. In our experiment, BEC is expected to first appear at the trap center when \( T \) is lowered from above \( T_c \) [26]. We thus compare the measured \( T_c \) with the critical temperature \( T_{c0} \) of a homogeneous lattice gas whose chemical potential matches that at the trap center. \( T_{c0} \) is obtained from a QMC approach [20] and we find \( T_{c0} = 6.3(3) J \), a value slightly shifted (\( \simeq 6\% \)) but compatible with \( T_c \). This observation suggests that our apparatus is suited to explore trap-size scaling and criticality [16, 30]. The direct measure of \( f_c \) also opens novel perspectives to investigate many-body quantum phase transitions, e.g. many-body localization in disordered lattices [33].

In conclusion, we have demonstrated to measure the 3D momentum distributions of interacting lattice gases with unprecedented accuracy and single-atom resolution. We have shown to estimate the temperature within a few % and to directly measure the condensed fraction. Thanks to single-atom resolution, the Helium detector can in principle access momentum correlations at any order. While its low detection efficiency (\( \simeq 25\% \)) could be a limitation, momentum correlations up to 6th-order were previously measured in ideal Bose gases [34]. In the future, it should thus be possible to probe multiple-particle correlations across quantum phase transitions, to allow for an experimental characterization of the many-body ground-state wave-function undergoing the transition [35] or to monitor the dynamics of momentum correlations after a quench [15].

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Experimental Sequence

Almost pure BECs of about $4 \times 10^4$ atoms in the state $2^3S_1$, $m_J = 1$ are initially prepared in a crossed optical trap (ODT) as described in [21]. We adiabatically load the BEC in the lowest energy band of an optical lattice made of three pairs of counter-propagating laser beams derived from a high-power laser source at telecom wavelength 1550 nm (Keopsys CEFL-KILO Series 15W). The lattice beams are turned on with a 100 ms-long exponential ramp with characteristic time $\tau = 20 \text{ ms}$. Meanwhile, the crossed dipole trap is switched off with an exponential ramp of duration 80 ms and $\tau = 20 \text{ ms}$. The final trapping frequencies are given by the gaussian shape of the lattice beams and equal to $\omega/2\pi \approx (308, 295, 298) \text{ Hz}$. In order to test the adiabaticity of the process we revert the loading procedure and check that the BEC possess no discernible thermal fraction.

The atoms are left in the optical lattice for a variable holding time (depending on the presence or not of the heating procedure) after which all laser beams are switched off and the cloud expands under gravity for a free fall of 50 cm. During the first 100 $\mu$s of expansion we rapidly transfer a variable fraction of atoms to the non-magnetic state $2^3S_1$, $m_J = 0$ with a resonant RF pulse ($\Delta E = h \times 6.8 \text{ MHz}$). We then apply a magnetic gradient to push the atoms remaining in the $m_J = \pm 1$ states away from the detector. The RF pulse power, combined with its time duration allows us to control the flux of atoms ($m_J = 0$) striking the detector. We typically operate between 1 and 50% RF transfer efficiency, the latter being chosen for the datasets at higher temperature ($T > 7J$) for which the atomic samples are more dilute.

Calibration of the single-atom Helium detector

The Helium detector is made of a pair of Micro-Channel Plates (Burle Industries, channel diameter 25 $\mu$m, center-to-center spacing 32 $\mu$m, angle of the channel $8^\circ$) mounted onto a crossed delay-line anode (Roentdek DLD80). The electronic pulses at the four ends of the delay line are amplified and converted into NIM pulses with dedicated constant fraction discriminators (Roentdek company). The digital coding of the arrival times of atoms ($m_J = 0$) striking the detector. We typically operate between 1 and 50% RF transfer efficiency, the latter being chosen for the datasets at higher temperature ($T > 7J$) for which the atomic samples are more dilute.

Reaching the far-field regime of expansion

To test the validity of the far-field approximation when using the Helium detector, we have investigated the time-of-flight dynamics of lattice BECs. The latter yields an interference pattern that can be pictured by considering the lengths $a$ and $L \gg a$ associated to the trapped BEC, giving rise to momentum components $k_a = 2\pi/a$ and $2\pi/L$ respectively. The momentum $k_a$ is associated with the distance between diffraction peaks in the interference pattern and $2\pi/L$ to the width of these peaks. As larger momenta develop faster during TOF, the diffraction peaks quickly separate. On the contrary, it takes longer for the width to establish. The far-field regime is reached when all momentum scales are fully developed, which happens after a TOF $t_{\text{FF}}$ that can be expressed in terms of the smallest momentum component, $t_{\text{FF}} = mL^2/2\hbar$ [17]. To monitor the relative dynamics of the momentum scales $2\pi/L$ and $k_a$, one can measure the ratio of the RMS peak size $\sigma$ to the peak-to-peak separation $d$ as a function of $t_{\text{TOF}}$. In far-field where the interference pattern is fully developed, the ratio $\sigma/d$ should be constant and proportional to $a/L$.

In the experiment, we let the the cloud expand for a
varying TOF and it is probed using two methods. At short TOF (from 2 to 20 ms) we take 2D absorption images. After a long TOF of 325 ms, we use the Helium detector. As shown in Fig. S1, we observe that $\sigma/d$ indeed saturates at long TOF, after a fast decrease at short TOF. In addition, we have further verified the variation with the system size $L$ (at fixed $a$) by increasing the atom number $N$ in the condensate to increase $L$. As expected, we observe that, the smaller the system size $L$, the faster the initial TOF dynamics and the larger the final value $\sigma/d$ (see Fig. S1). For $N = 4 \times 10^4$ atoms we find that $t_{FF} \approx 50$ ms is much shorter than $t_{TOF} = 325$ ms, indicating that the distributions measured by the Helium detector is in far-field.

**Heating sequence**

To vary the temperature in the lattice, we have used a controlled heating sequence. After loading the BEC in the lattice, a series of non-adiabatic pulses of 0.5 ms duration each is performed with one of the lattice beams. The number of pulses (from 5 to 10) and their amplitude $V_{\text{heat}}$ are varied to obtain different final temperatures in the lattice while keeping the number of atoms constant. After the pulse sequence, the cloud is left to thermalize for a time interval of 40 ms ($\sim 20 \ h/J$). By exploiting a band mapping technique we have verified that no discernible fraction of atoms is transferred to higher lattice bands.

**QMC calculations**

Exact thermodynamic properties of interacting lattice bosons can be studied using Quantum Monte Carlo (QMC) methods. In this work we have used the worm algorithm QMC, following the scheme of Pollet et al. [S1].

The main idea of this approach is to consider a stochastic representation of the partition function $Z = \text{Tr}[e^{-\beta H}]$, with $\beta = 1/k_b T$ is the inverse temperature, and $H$ is the Bose-Hubbard Hamiltonian. The starting point is to decompose the Hamiltonian into two terms: $H_0 = \frac{U}{2} \sum_i n_i(n_i - 1) + V_{\text{trap}}$ and $H_1 = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \text{h.c.}$, and consider the Dyson series for the partition function:

$$Z = \sum_{n=0}^{\infty} (-1)^n \int_{0<\tau_1\leq\ldots\leq\tau_n<\beta} d\tau_1 \ldots d\tau_n \text{Tr} e^{-\beta H_0} H_1(\tau_n) \ldots H_1(\tau_1),$$

where $H_1(\tau) = e^{\tau H_0} H_1 e^{-\tau H_0}$ is the time-evolved $H_1$ in the interaction representation. Each of the terms in the Dyson series are then sampled stochastically, using an extended configuration space including open world lines (the so-called “worm”).

This approach also allows to measure efficiently the equal-time, two-particle Green function $g_{lm} = \langle b_i^\dagger b_m \rangle$, for pairs of sites $l$ and $m$. The momentum distribution for the trapped system is then obtained as:

$$n(\vec{k}) = |w(\vec{k})|^2 S(\vec{k}),$$

where $w(\vec{k})$ is the Fourier transform of the Wannier function associated to the optical lattice, and

$$S(\vec{k}) = \sum_{lm} g_{lm} e^{i \vec{k} \cdot (\vec{R}_l - \vec{R}_m)},$$

where $\vec{R}_l$ denotes the coordinate of the $l$-th lattice site. In our simulations, we have fixed the total chemical potential in the system in order to match the estimated experimental value for the total number of particles in the system.

For the homogeneous lattice gas (i.e. in the absence of a trapping potential, and considering a cubic box with periodic boundary conditions) we have determined the transition temperature $T_c$ for the superfluid transition through the winding number estimator of the superfluid density [S2]. In this case the chemical potential has been fixed to match the chemical potential estimated at the center of the trap for the experimental configuration. Our calculations were performed using an updated version of the DWA code in the ALPS library [S3, S4].

**Extracting the condensed fraction $f_c$**

As explained in the main text, the inequality $L \gg a$ allows us to distinguishing the condensate contribution

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**FIG. S1.** Reaching the far-field regime during the TOF expansion of lattice superfluids. Time evolution of the width $\sigma$ of the diffracted peaks normalized to the peak distance $d$. Data sets with a varying total atom number $N$ correspond lattice superfluids with different in-trap size $L$. Solid lines are a guide to the eye.
\( n_0(\vec{k}) \) from that of the depletion \( n_{NC}(\vec{k}) \). The condensate \( n_0(\vec{k}) \) consists in sharp peaks of size \( \propto 1/L \) and measuring the condensed fraction \( f_c \) thus amounts to measuring the atom number \( N_{\text{peak}} \) in the condensate peaks with respect to the total atom number \( N \), \( f_c = N_{\text{peak}}/N \). Here we make the assumption that \( N_{\text{peak}} \approx N_0 \) with \( N_0 \) the number of condensed atoms and \( N = N_0 + N_{NC} \). This also relies on the inequality \( a/L \ll 1 \) which ensures that the fraction of depleted atoms contained in the sharp peaks is extremely low, of order \( (a/L)^3 \).

To identify the momentum \( k_0 \) which delimits the two contributions to \( n(\vec{k}) \) we focus on the first diffracted peak that is not affected by saturation effects of the detector. We fit 1D profiles with a Gaussian centered at \( k = k_a \) on top of a power-law. We defined \( k_0 \) as the momentum where these two fitted distributions intersect, as illustrated in Fig. S2(a). The large dynamical range in density provided by the Helium detector is of primary importance to accurately fit the tails associated to the depletion of the condensate and identify \( k_0 \) accurately. A similar approach would result difficult from column-integrated images as obtained when probing quantum gases with absorption imaging. In Fig. S2(b), we plot \( k_0 \) as a function of the temperature \( T \). For \( T > T_c \), one can not identify a double structure with an abrupt change of slope (see experimental profiles at \( T = 7.2 \, J \) in Fig. 3) and we set \( k_0 = 0 \).

Since the momentum distribution is translation invariant (up to an envelop factor given by the Fourier transform of the Wannier function), we extract \( f_c \) by considering a single Brillouin zone only. In the 3D distributions, we count the atom number in the central peak \( N_{\text{peak}}^0 \) and the atom number in the first Brillouin zone \( N_{BZ} \). To take into account the saturation of the detector around \( k \approx 0 \), the measured atom number in the central peak is multiplied by a scaling factor \( \alpha \) obtained from the amplitude of the first-order diffracted peak, \( \alpha = n(k_a, 0, 0)/[\tilde{\omega}(k_a) \cdot n(0, 0, 0)] \). We then calculate \( f_c = \alpha \cdot N_{\text{peak}}^0 / N_{BZ} \).

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