Spatial tomography of individual atoms in a quantum gas microscope

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We demonstrate a method to determine the position of single atoms in a three-dimensional optical lattice. Atoms are sparsely loaded from a far-off-resonant optical tweezer into a few vertical planes of a cubic optical lattice positioned near a high-resolution microscope objective. In a single realization of the experiment, we pin the atoms in deep lattices and then acquire multiple fluorescence images with single-site resolution. The objective is translated between images, bringing different vertical planes of the lattice into focus. In this way, we tomographically reconstruct the atom distribution in three dimensions. This opens up the possibility of extending the domain of quantum simulation using quantum gas microscopes from two to three dimensions.

It is becoming increasingly clear that a complete understanding of quantum materials requires an understanding of phenomena like correlations, fluctuations and entanglement down to the single-particle level. Neutral atoms are among the prime candidates for performing scalable quantum simulations and there are currently two main platforms for pursuing this.

The first of these relies on the usage of multiple tightly focused optical tweezers directly loaded with atoms from a magneto-optical trap [1, 2]. As a result, the atoms are typically not in the motional ground state, and the inter-atomic couplings are mediated by Rydberg interactions. Tweezer-trapped atoms can, however, be cooled to the ground state [3, 4], and this enables tunnel-coupling between adjacent tweezers [5, 6]. Large arrays of ground-state cooled single atoms have recently been realized, demonstrating the scalability of these systems [7, 8].

A second platform studies ultracold atoms loaded into the ground state of wavelength-scale optical lattices by means of high-resolution microscopy in so-called quantum gas microscopes (QGMs) [9, 10]. Both of these platforms offer a high degree of control and tunability [11]. The work presented here combines aspects of both methods.

Quantum gas microscopes operate in a regime where a short lattice spacing allows for tunnel coupling between atoms in adjacent potential wells. These systems have proven to be especially useful for quantum simulation of many-body systems [12]. Prominent applications in bosonic systems include the study of 1D Heisenberg spin-chains [13], quantum random walks [14], the links between mixed quantum states and thermal ensembles [15], and the realization of many-body localized states [16]. One of the biggest advantages of QGMs is direct access to high-order particle-particle correlations, which are essential for the description of many-body quantum states. The construction of fermionic QGMs [17, 19] enabled the study of quantum magnetism which relies heavily on such correlations. Measurements of correlations both in the spin and charge sectors have revealed long-range anti-ferromagnetic ordering in 2D systems [20], hidden anti-ferromagnetic correlations in 1D Heisenberg spin-chains [21], and have been central to the continued development of our understanding of intriguing phenomena such as superconductivity at high temperatures [22, 23].

With the exception of one study on a bilayer Mott insulator [24], investigations with QGMs have been constrained to physics in one or two spatial dimensions due to imaging limitations. Full 3D tomography has only been demonstrated in large-spacing lattices [25] and in 3D arrays of optical tweezers [26], where the spacing between atom layers is an order of magnitude larger than that of the system reported on here.

In this article we present a novel method for the tomographic reconstruction of the 3D distribution of ul-
tracold $^{87}\text{Rb}$ atoms sparsely populating a cubic optical lattice potential. Our experimental apparatus is a QGM of the type presented in Refs. [9]–[10]. A schematic of the experiment is shown in Fig. [1]. The atoms are placed within the (dynamically translatable) focus of a microscope objective with a numerical aperture (NA) of 0.69. By pinning the atoms in a deep optical lattice, we can use high-contrast fluorescence imaging to determine the atoms’ position to within a single site of the lattice. The microscope objective is mounted on a piezo-driven objective scanner with a scan range of 400 µm, which enables control of its vertical position to nanometer precision. It is this vertical control that allows us to perform tomographic scans. Within a single realization of the experiment, we acquire multiple fluorescence exposures, where the position of the microscope objective is translated between images. Thus, we can extract an atom’s position not only in the two horizontal dimensions but also along the (vertical) line-of-sight. This method demonstrates a step towards investigations of many-body physics with QGMs in three dimensions.

The full experimental sequence proceeds as follows: initially, atoms are loaded into a magneto-optical trap and subsequently transferred to a magnetic quadrupole potential. The atoms are then cooled by forced evaporative cooling methods as detailed in Refs. [27]–[29] and held in a crossed optical dipole trap at a wavelength of 1064 nm. This results in a cold cloud of about $10^6$ atoms at an approximate temperature of 800 nK. The atoms are then loaded into a 940 nm optical tweezer potential generated by directly imaging the pattern displayed on a digital-micromirror device (DMD) through the microscope objective onto the atoms. The resulting tweezer has a $1/e^2$ waist of 780(20) nm. To sparsely load atoms into the lattice, the tweezer depth is set to 20 nK, such that the atoms are merely levitated against gravity. The atoms are then loaded into the vertical lattice and allowed to diffuse within their respective lattice planes. Subsequently the two horizontal lattice axes are ramped on, and the atoms are frozen in a cubic lattice with a depth of 2000 $E_r$, where $E_r = h^2/2m\lambda^2$ is the recoil energy, $m$ is the mass of the atom, and $\lambda = 1064$ nm is the wavelength of the lattice light. The atoms are then exposed to molasses light configured as in Ref. [10], and their fluorescence is captured by the objective and recorded on an EMCCD camera. A typical experimental image is shown in Fig. 2(a).

To identify atoms, a peak-finding algorithm is applied to all the images. In order to determine the resolution of our imaging system, we superimpose 20 of the brightest signals from the image shown in Fig. 2(a), where the atoms’ centers are determined by a 2D Gaussian fit applied subsequent to the peak finding. In this way we create an averaged image of an atom, as shown in Fig. 2(b). A horizontal cut through the image is fit with a 1D Gaussian as shown in Fig. 2(c) and used to determine the resolution limit given by the Rayleigh criterion, resulting in $r_{\text{min}} = 713(14)$ nm, in accordance with the manufacturer’s specifications.

In order to tomographically reconstruct the position of an atom along the vertical lattice planes, we measure its intensity as a function of the objective position. To obtain the data presented here, the atoms were imaged in five 200 ms long exposures separated by the same amount of time. During the separation time the objective was translated through a set of positions $\{z_k\}$, where $k = \{-2, \ldots, 2\}$, spanning a total range of 2 µm. Figure 2(d) shows raw and low-pass filtered images of the same atom obtained in this manner. The light intensity scattered by the atom increases up until the fourth image, where the atom is in focus, and then decreases in the fifth image as the atom moves out of focus. This information can be used to pinpoint into which plane along the line-of-sight the particular atom was loaded.

The experiments are subject to moderate heating effects. The atom loss (and thermal hopping) during the imaging procedure mainly stems from heating along one of the axes of the optical lattice and the fact that our molasses beams do not cover the entire atom cloud. Therefore we lose approximately 25% of our atoms over the

![Figure 2. Fluorescence signals from single atoms. (a) An image of about 40 atoms. From the atom in the inset we collect approximately 8000 photons in total. (b) The 20 brightest signals in (a) are superimposed to create an averaged image. (c) A horizontal cut through the averaged image is fit by a Gaussian function (blue, dashed). The simulated PSF as provided the manufacturer is also plotted (orange, solid). (d) A series of five fluorescence images of a single atom, where the microscope objective was translated by 0.5 µm between consecutive shots. (left column) Raw data. (right column) Data treated with a low-pass filter. The numbers to the right mark the position of the objective, referenced to the center position of the series of images.](image-url)
FIG. 3. Determination of an atom’s vertical lattice plane. (a) Atomic fluorescence signal measured in terms of the PTR plotted as a function of the relative objective position $z$ and corresponding parabolic fits (see main text). The four traces correspond to atoms loaded into planes $k = -1$ (yellow diamonds, dash dotted line), $k = 0$ (red squares, dotted line), $k = 1$ (purple triangles, dashed line), and $k = 2$ (blue circles, solid line). (b) Histogram of the experimental atom signals as a function of $\Delta z$, the distance of the objective focal position to the lattice plane in which the atom was loaded. (c) Histogram of simulated data using Fresnel propagation. The color in (c) has been chosen to match the experimental data.

As shown in Fig. 2(d), atoms out of focus will appear fainter and cover a larger area than those in focus. As a measure of this effect we introduce the peak-to-total ratio (PTR) corresponding to the ratio of the photon count $N_{3\times3}$ in a $3 \times 3$ pixel array around the center of the atom image to the photon count $N_{7\times7}$ in a $7 \times 7$ pixel array around the center (chosen because 7 pixels corresponds to $r_{\text{min}}$),

$$\text{PTR} = \frac{N_{3\times3}}{N_{7\times7}}. \quad (1)$$

For each static atom, we calculate the PTR using the filtered version of the image as a function of the objective position, as shown in Fig 3(a). In order to interpret this data, we consider how the atom image diffracts as the objective is moved. The axial intensity of the point-spread function (PSF), $I_{\text{PSF}}$, is given by [30]

$$I_{\text{PSF}}(z) = I_0 \sin^2(\xi z), \quad (2)$$

where $I_0$ is the peak intensity and $\xi = \frac{\pi}{\lambda} N A^2$. A Taylor expansion of $I_{\text{PSF}}$ around the origin yields an inverse parabola.

Thus, we can fit the PTR of each atom as a function of the objective position with an inverse parabola with a fixed curvature [31], also shown in Fig 3(a). As a next step, we compile a histogram of the PTR for each value of $\Delta z$, as shown in Fig 3(b). Here, $\Delta z = z_k - z_{\text{fit}}$, where $z_{\text{fit}}$ corresponds to the lattice plane to which each trace was fitted. This centers the traces around the vertical lattice plane into which the respective atom was loaded. These results are compared to simulated data (including photonic shot noise, coma in the imaging system, and random technical noise) generated using Fresnel propagation and analyzed in the same way. The simulated data, shown in Fig. 3(c), reproduces the experimental results very well, confirming our analysis.

Importantly, this analysis allows us to find the vertical distribution of the atoms, as displayed in Fig 4(a), which shows a histogram of the population fraction loaded into a given plane. It is important to note, however, that some of the (very few) atoms loaded into the $\pm 2$ lattice planes are neglected in our current implementation of the method, as those atoms’ signals fall below the imaging noise floor in subsequent images and are thus not detected in all five images. In future work, this can be easily remedied by taking images that span more than five lattice planes.

Furthermore, the total measured light intensity should be equal to the sum of individual $I_{\text{PSF}}$ contributions (cf. Eq. 4) from each lattice plane. Given the relative population $p_k$ of atoms in the planes from Fig 4(a), we define a total intensity $I_{\text{tot}}(z)$ as

$$I_{\text{tot}}(z) = \sum_k p_k I_{\text{PSF}}(z - k \lambda / 2). \quad (3)$$

The average total number of photons collected per atom
FIG. 4. Atom population in the lattice planes. (a) Histogram of the relative population detected in each lattice plane for the atom traces considered in this work. (b) Reconstruction of the photon count $N_{7\times7}$ per atom per plane as a sum of atom intensities detected in the separate planes, i.e., the different terms in Eq. (3) (solid lines).

is plotted in Fig. 4(b). Equation (3) is fit to the data, where the only free parameter is the overall intensity $I_0$ in Eq. (2). This simple treatment matches the measurements, providing further evidence for the veracity of our method, and also shows that our loading procedure resulted in a narrow range of loaded lattice planes.

Finally, we tomographically reconstruct the 3D spatial distribution of all of the atoms analyzed, as shown in Fig. 5. The vertical distribution is obtained from the fitted position $z_{fit}$ of each atom. The horizontal position of the atom is determined by matching its lateral position in the first image of the trace to the nearest lattice site. While this image uses atoms drawn from a series of experimental runs, with improved molasses cooling and better stability of the optical lattices, nothing fundamentally prevents the determination of the full atom distribution within a single experimental realization.

Our tomographic approach faces obvious experimental challenges when it comes to imaging dense samples in multiple planes, such as precisely determining the location of holes in a multi-layer Mott insulator. However, such tomography in dense samples is not excluded and could indeed allow for more precise determination of the superfluid-to-Mott-insulator transition in three dimensions. Currently the strength of our method lies in the analysis of sparsely-filled systems distributed over a handful of lattice planes along the line-of-sight.

This method could be applied to study a broad class of transport problems in three dimensions, including spintronics, light-harvesting systems, or the spreading of impurities in a spin system. One particular experiment that fulfills the condition of sparse loading is the realization of quantum random walks in 3D, which has been investigated before in 1D with QGMs and in photonic systems. To study interesting dynamics in this setting one could, for example, tilt the lattice (which is already a non-trivial classical problem) or modulate it to study diffusion of higher motional states.

Most importantly, our method allows for three-dimensional quantum simulations that explore the difference between bulk and edge effects in solid-state systems (including topological insulators). For example, an isolated system of $n_x$-by-$n_y$-by-$n_z$ atoms could be prepared by a combination of DMD projected potentials and horizontal light sheets. This would enable the study of dynamics such as many-body entanglement and localization. To preserve the sparse conditions under which tomographic imaging is favorable, the system could undergo dynamics and subsequently be allowed to spread in the lattice before imaging, as is already done in QGMs. In this new regime of quantum simulation, the dimensionality of the system renders numerical simulation of the system difficult.

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