Efficient preparation of 2D defect-free atom arrays with near-fewest sorting-atom moves

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Sorting atoms stochastically loaded in optical tweezer array via an auxiliary mobile tweezer is an efficient approach to prepare defect-free atom arrays of arbitrary geometries. However, the filling fraction of atom-by-atom assemblers is impeded by redundant sorting moves with imperfections during atom transport, especially for scaling the system size to larger atom numbers. Here, we propose a new sorting algorithm (heuristic cluster algorithm) which provides near-fewest moves in tailored our atom assembler scheme and experimentally demonstrate a 5 × 6 defect-free atom array with 98.4% filling fraction for one rearrangement cycle. Furthermore, the novel feature of this algorithm makes the filling fraction high and uniform as the size of atom assembler enlarged. Our approach is essential to scale hundreds of assembled atoms for bottom-up quantum computation, quantum simulation and precision measurement.

INTRODUCTION

Bottom-up builded single atom arrays have rapidly developed into a versatile platform for quantum many-body simulation [1–4], quantum metrology [5, 6] and quantum computation [7–12]. Several crucial advantages of this system have been experimentally demonstrated, besides configurable defect-free atom arrays via atom rearrangement [13–18], long coherence time of quantum bits (qubits) well-isolated from environment [5, 19–21] and controllable long-range interactions using Rydberg atoms [22–25]. Since a great amount of quantum science and technology based on assembled-atom platforms will strongly benefit from scaling the system size to larger atom numbers such as building an fault-tolerant information processor with sufficient logic qubits to solve classical untractable tasks [26]. However, determined preparing hundreds of atoms with full control over spatial geometries is still a challenge.

Recent years, the atom-by-atom assemblers have been scaled from one dimension to three dimension [27, 28], meanwhile the array size has been increased to about two hundred atoms [29]. An effective and conventional approach to achieve the defect-free atom arrays of arbitrary geometries is sorting randomly distributed atoms to target sites via an auxiliary mobile tweezer (MT) [15, 18]. The filling fractions of the final atom arrays are closely related to atom transfer efficiency to target sites. Because the failure of extracting atoms out by a MT makes the atoms stay in situ and may cause collisional loss in next transfer process. Moreover, the atom loss in the MT and the imperfect of releasing atoms into target sites lead to defects in final atom arrays. To increase the filling fraction, an optimal sorting path with fewest number of sorting moves can minimize the influence of the imperfection during the atom rearrangement. Thus, finding an atom sorting algorithm well suited for large scale defect-free atom assemblers is essential.

Heuristic shortest-move algorithm has been applied to rearrange atoms and the cumulative success rate of a 4 × 4 atom array is less than 20% for one rearrangement cycle mainly limited by a 75% transfer efficiency (might be induced by the short lifetime in the MT) [18]. A similar sorting algorithm called heuristic path-finding algorithm (HPFA) is chosen to prepare a 5 × 5 atom array with a filling fraction of 96% [15]. However, these sorting algorithms are not appropriate for large scaled atom arrays due to a number of redundant moves involved in. Here, we propose a heuristic cluster algorithm (HCA) which significantly reduces the number of moves for sorting atoms and demonstrate it experimentally by preparing a 5 × 6 atom array with 98.4% filling fraction (after correcting the 4% atom loss due to the background gas collisions and the loss during the probing atom process) for one rearrangement cycle.

We begin by introducing an 8 × 8 atom array setup. Then, we improve the atom lifetime in the MT and prove that no obvious atom loss is observed when a atom is transferred across optical tweezer array in a relatively long move distance. In this case, a sorting algorithm provides fewest moves is preferred. Next, three sorting algorithms are briefly described and compared. Finally, we experimentally measure the filling fraction of atom arrays utilizing these algorithms with two different transfer efficiency and give simulating results for large scaled atom arrays.
FIG. 1. (color online). Images of 2D defect-free atom arrays. (a) Loading rates histogram of 64 tweezers. The average loading rate of 64 tweezers is 53% measured by 200 times repeating loading process. (b) Fluorescence count distribution for 64 tweezers during 80 ms of exposure after 200 times loading process. The region of interest for each tweezer is $2 \times 2$ pixels. (c) Schematics of the experimental setup. (d) Determined preparing a filled tweezer in target sites via transporting a single atom (blue disk) from another filled tweezer with the MT. This process represents one move. (e) Defect-free atom arrays in the specific patterns of capital English letters via atom rearrangement. The unused extra atoms are discard by moving them to positions far away from the field of view. The distance between neighboring atoms is 5 $\mu$m.

EXPERIMENTAL PREPARATION OF ATOM ASSEMBLERS

The $8 \times 8$ optical tweezer array is generated by an 808 nm laser beam deflected in two orthogonal directions by a dual axis acousto-optic deflector (AOD). The dual axis AOD are respectively driven by two radio-frequency (RF) signals with 8 tones (the central frequency is 96 MHz and the frequency gap between the neighboring tones is 2 MHz) which is produced by an arbitrary waveform generator (AWG, Keysight M3202A). The optical homogeneity of the trap array is less than 10% after optimization. The 830 nm MT is also created by an AOD with the RF signal sent from a voltage controlled oscillator (VCO, Mini-circuits ZOS-150+) with the frequency tuned by a direct current (DC) voltage. The Gaussian waist of the each tweezer in the array and MT are both about 1.0 $\mu$m. Our experimental setup is shown schematically in Fig. 1(c).

Single $^{87}$Rb atoms are stochastically loaded from a magneto-optical trap into optical tweezer arrays with trap depth of $U_0/k_B \approx 0.8$ mK for each tweezer in 950 ms, where $k_B$ is the Boltzmann constant. The photoelectron count threshold and the regions of interest for every tweezer are periodically calibrated by a computer program via automatically analyzing a series of atom array images. Images of atom fluorescence are taken by an electron multiplying charge coupled device (EMCCD) camera (Princeton Instruments ProEM+:1024B). Fig. 1(a) and Fig. 1(b) respectively illustrate the loading rates and the average threshold of 64 sites. Next, atoms in reservoir tweezers are transferred to the target sites using a MT in a real time sorting path calculated by sorting algorithm. The sorting path is composed of three waveforms to control the intensity and X and Y positions of the MT respectively. For the rearrangement process as depicted in Fig. 1(d) we spend 1 ms adiabatically increasing the trap depth of the MT to 2.3 mK after the MT overlaps a filled reservoir tweezer. Then, the MT extracts the atom out and moves at the speed of 1 ms/grid (one grid represents the distance between two neighboring sites) across void tweezers to the target site. After the atom in the MT released into the target site in 1 ms, the next rearrangement cycles for other target sites are carried out. Finally, we acquire a new image to reveal the new positions of the atoms in the array as shown in Fig. 1(e). The total rearrangement time is less than 80 ms for a $5 \times 6$ atom assembler.

ATOM LIFETIMES IN A MOBILE TWEEZER

In order to optimize the filling fraction of defect-free atom arrays, we firstly improve the atom lifetime in a MT because the atom loss directly leads to the defects in the final atom arrays. As described above, the position of the MT is controlled by the frequency of RF signals which are sent into the AOD. We experimentally find that the atom lifetime is affected by the beam-pointing fluctuations of the MT [30]. The beam-pointing noise observed by the
also be suppressed by the continuous laser cooling. The reduction atom lifetime to 2.1 s, but this heating effect can interfere between neighboring tweezers in the array. We note that another heating effect due to the light of 2.27 mK, 0.82 mK, 0.77 mK and the trap depth of void tweezers is 0.8 mK.

FIG. 2. (color online). Atom lifetimes in a MT. (a) Atom survival probability is in a static MT. The orange circles, red squares and purple diamonds are respectively denote the lifetime with RF driver generated by three approaches. The first manner is that the RF signals come from a signal generator (Agilent E4433B, the deviation of frequency modulation is 5 MHz/V) with frequency modulated by a DC voltage sent from an analog output (National Instruments PXI-6733). In the second manner, a purer DC voltage is generated by an AWG (Keysight 33522A) instead of the analog output. For the third one, VCO produces the RF signals tuned by DC voltage output from the AWG. The solid curves are fitted to Eq. (1) and heating rates are 30/s (orange circles), 3.9/s (red squares), 0.32/s (purple diamonds). The inset illustrates the frequency spectrum of the RF signals. The sidebands are induced by the noise of the DC voltage to control the RF frequency in the mode of frequency modulation. (b) Atom survival probability in a MT after transferred across several void tweezers in the array. The black squares, blue triangles, red circles respectively represent the results with the MT depth of 2.27 mK, 0.82 mK, 0.77 mK and the trap depth of void tweezers is 0.8 mK.

Sideband of the RF signal frequency spectrum causes a heating effect when the noise frequency is about 90 kHz (equal to the atom oscillation frequency in the harmonic trap). Since the heating rate is constant, the survival probability of atom in MT as the function of time can be expressed as [31]

$$P_s(t) = 1 - \left[ 1 + \frac{1}{\nu t} + \frac{1}{2(\nu t)^2} \right] e^{-\frac{t}{\nu t}},$$

where $t$ is the atom hold time in MT and $\nu$ is the heating rate leading to atom loss. We measure the atom lifetime in a static MT with RF signal of different frequency spectrum and conclude that the lifetime depends on the amplitude of the sidebands (about 90 kHz detuning from the carrier) as depicted in Fig. 2(a). Moreover, the lifetime is further increased to 7 s when we apply continuous laser cooling (turning on repump light resonant with $|5s_{1/2}, f = 1\rangle \rightarrow |5p_{1/2}, f = 1\rangle$) and cooling light red detuned by 24 MHz-54 MHz from $|5s_{1/2}, f = 2\rangle \rightarrow |5p_{3/2}, f = 3\rangle$ simultaneously. Additionally, we should note that another heating effect due to the light interference between neighboring tweezers in the array reduces atom lifetime to 2.1 s, but this heating effect can also be suppressed by the continuous laser cooling. The cooling process however will destroy the internal state if the atoms are encoded into qubits, thus our work that atom lifetime is improved in a MT without cooling is still necessary.

Furthermore, the atom survival probability in the MT is measured after the MT moves across several void tweezers as shown in Fig. 2(b). We observe that it decreases as the number of void tweezers is increased when the MT depth is less than or approximately equal to the depth of each void tweezer. However, atoms are preserved well when the MT depth is sufficiently deep. Therefore, we tend to choose a sorting algorithm with fewer moves in tailored our atom assembler scheme and the move distance is not taken into the main consideration.

**SORTING-ATOM ALGORITHMS**

Now, we introduce the sorting atom process of HCA, ASA and HPHA respectively as sketched in Fig. 3. HCA, aiming at costing the number of moves as few as possible are proposed to find smart sorting path to fill empty target sites with source atoms in reservoir traps. We define the reservoir tweezers as the outside-region and all target sites as the inside-region. To achieve the goal with near-fewest moves, we try not to move the atoms in inside-region, which also means target sites should be directly filled with source atoms in outside-region instead of the atoms in inside-region. The first step of HCA is to identify the “closed-region” and the “open-region” of the initial atom array. The closed-regions are the two orange sections which are isolated from the outside-region and the open-regions are the three blue sections adjacent to the outside-region. The number of moves to fill the open-region can be equal to the empty target sites which is also the fewest. But the closed-regions can not directly obtain source atoms due to the obstacle atoms. Thus, filling the empty target sites in closed-region takes more moves than the cost in open-region. The core ideal of HCA is to convert the close-regions to open-regions. Then, obstacle atoms (in dash circle) that block the connection between the closed-regions and the open-regions are moved to the closed-regions to open the closed-regions. The obstacle atoms are searched around the open regions site by site (sometime, more than one atom should be moved to open up the close regions). After that, all regions are open and filled with the source atoms in order (the site with the longest distance from the outside-region filled first).

ASA is another sorting algorithm that fills the empty target sites from the center to the edge with two main steps. The first step is to find the center location of the atom array and classify the layers (section in the blue, orange and red dash line square) in inside-out order. The second is to fill the trap, one layer after the other. Tweezers of target sites adjacent to the reservoir tweezers are defined as the first layer. The second layer contains
the sites in inside-region adjacent to the first layer. The classifying layer process continues until no new layer can be found. The last one is the center of the atom array. Usually, since filling from the center significantly reduce the sorting moves, this is the reason why we classify the layers. In the second step, ASA fills the layer one by one in the reverse order of layers. The search source atom process is similar to A* searching algorithm (finding the nearest atom and moving it bypassing the obstacles to the target site in the shortest path).

Compared with the HPFA in Ref. [15], our HPFA does a certain amount of optimization. The upgraded HPFA does not calculate all the distance between each atom and each target tweezer. Instead, we define a parameter named search distance which is set to be one at the beginning. We check all the empty tweezer whether there are atoms in the reservoir tweezer satisfied with the search distance. If the choices are multiple, we will select the one which has the least obstacle atoms in the sorting path to achieve as few moves as possible. If there is an “obstacle” atom blocking the sorting path, we move this atom to the target site and replace the obstacle by a source atom. The search distance is continuously increasing un-

![Diagram](image)

FIG. 3. (color online). Schematic diagrams and flowcharts of HCA, ASA and HPFA. The sorting process is from left to right.

**NUMBER OF MOVES AND FILLING FRACTIONS**

All these three sorting algorithms seem feasible and effective to prepare 2D defect-free atom arrays of small size, however their costs of transfer moves and distance are different especially when the atom size is increased. As simulating results, HPFA provides the shortest transfer distance (see Fig. 3(a)) but costs the most transfer moves (see Fig. 3(b)). In contrast, we adopt HCA with the fewest transfer moves at the expense of the longest transfer distance. Since the transfer distance has no obvious relation to the filling fraction of the final atom arrays, HCA should be a better sorting algorithm compared to HPFA and ASA as seen Fig. 3(c). Additionally, we note that transfer time is also a main factor to affect the filling fraction because of the atom loss in tweezer array limited by the lifetime. For example, if we prepare a 30 \times 30 atom array (the details of transfer process has been described above), ASA, HCA and HPFA respectively take 6.7 s, 8.2 s and 9.6 s. This indicates ASA may be the best choice when transfer time dominates the filling fraction. Our time-dependent transfer process is not optimal and we do not take the transfer time into account when selecting a sorting algorithm, because we have not implemented the fast and adiabatic transport approach yet which can significantly reduces the time cost [32, 33].

Furthermore, we experimentally measure (see Fig. 3(d)) and simulate (see Fig. 3(e)) the filling fractions \( \eta \) of defect-free atom arrays using these three sorting algorithms. The \( \eta \) is given by \( \eta = 1 - n(1 - \zeta) \), where \( \zeta \) is the transfer efficiency and \( n \) represents the move number per one filled target site. Although the distinction of the filling fraction is small when the transfer efficiency is high and the array size is not large, the sorting algorithm with fewer \( n \) demonstrates obvious advantage as the transfer efficiency is decreased or the array size is enlarged. Additionally, we find that the filling fractions with HCA and ASA are almost constants as filled site number increased, while HPFA shows a rapidly decline. Thus, HPFA is not appropriate for large scaled atom arrays even with a high transfer efficiency. The cumulative success rate of the final atom assembler is shown as Fig. 3(f).

Although finding the optimal sorting path is a difficult computational task (likely to be a NP-complete problem), the newly proposed HCA with the near fewest sorting moves provides a better choice than other sorting algorithms as demonstrated by experimental and simulation results. There are still some experimental imperfections which should be improved. The tweezer array generated by our scheme can be scaled to \( 32 \times 32 \) sites as shown in Fig. 1(c), but the size of atom array is limited.
FIG. 4. (color online). Number of moves of HCA, ASA and HPFA and filling fractions of the defect-free atom array as the number of filled sites. (a) Simulating results of the transfer moves as the function of filled site numbers. (b) Simulating results of the transfer distances as the function of filled site numbers. The error bars are caused by the randomly distributed initial atom arrays with 50% loading rate. The shape of the target sites are all squares. (c) Histogram of the number of moves to prepare a 14 × 14 square array for 10000 initial random loading instances. (d) Experimental filling fraction of atom array after atom rearranged by ASA, HCA and HPFA. The solid line and the dash line respectively represent the experimental results in the condition of 97.7% and 88.0% transfer efficiency (the average values for 64 sites). The lower transfer efficiency is obtained by the position displacement of MT and tweezer array. (e) Simulating filling fraction of large scaled atom array using ASA, HCA and HPFA. The solid line and the dash line respectively represent the simulating results in the condition of 99% and 90% transfer efficiency. (f) Simulating cumulative success rate (\(R_c = \eta^N\)) of the final atom array as the number of filled sites with 99% transfer efficiency.

by the optical power of 808 nm laser beam for reliable atom loading. The filling fraction decays as the filled sites number increased mainly induced by the nonuniform transfer efficiency of 64 sites (the efficiency of transporting atoms to the edge sites in atom array is lower than the transfer efficiency to the center sites). Except for the 4% atom loss limited by the atom lifetime in tweezer array, to obtain higher filling fraction we should make the MT and every site in tweezer array overlap perfectly in both radial and longitudinal directions during the atom rearrangement.

CONCLUSION

In conclusion, to improve the filling fraction of defect-free atom array, we develop a sorting algorithm (HCA) which significantly reduces the redundant sorting moves. We experimentally proved the advantage of HCA over other sorting algorithms. The novel feature of HCA is the high and uniform filling fraction as the size of atom assembler increased. This property makes our approach well suited for quantum simulation of quantum dynamics [34] and gauge theories [35], error-corrected quantum computation [36, 37], single molecule arrays [38–40] and quantum metrology based on large scale reconfigurable atom arrays.

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preparing enhanced atom-by-atom assembly [41].

Note added.-Recently, we became aware of related work preparing enhanced atom-by-atom assembly [41].
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