

Initializing a quantum register from Mott-insulator states in optical lattices

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We propose and quantitatively develop two schemes to quickly and accurately generate a stable initial configuration of neutral atoms in optical microtraps by extraction from the Mott-insulator state in optical lattices. We show that thousands of atoms may be extracted and stored in the ground states of optical microtrap arrays with one atom per trap in one operational process demonstrating massive scalability. The failure probability during extraction in the first scheme can be made sufficiently small ($\sim 10^{-4}$) to initialize a large-scale quantum register with high fidelity. A complementary faster scheme with more extracted atoms but lower fidelity is also developed.

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Introduction. Neutral atoms are well isolated from the environment and may offer a route to scalable quantum computation. Different neutral-atom quantum computing proposals [1–3] differ in trapping techniques. We focus on arrays of microscopic traps (microtraps) that can be implemented using independent focused laser beams. The typical size of a microtrap in current experiments is about $2\ \mu\text{m}$ because of the diffraction limit of a laser beam as well as experimentally technical issues. Unlike an optical lattice, all microtraps can be moved independently in position space; therefore, they have advantages in single atom addressability and controlled interactions between pairs of atoms. In recent years, many schemes have been proposed for universal quantum computation in microtrap systems [3].

These schemes are based on the assumption that thousands of neutral atoms can be prepared in the ground states of optical microtrap arrays with one atom per trap; i.e., they assume the ability to initialize a neutral-atom quantum register. Although impressive experimental progress has been made in trapping single atoms [4], such an assumption has not been fulfilled because the trapping processes are random and not deterministic. Furthermore, the trapped atoms are not in the trap ground states. These difficulties have prevented neutral-atom quantum computation architectures from accomplishing the kind of impressive experimental progress recently achieved in ion-trap quantum computation [5]. To overcome these difficulties one proposal seeks to extract single atoms from a Bose-Einstein condensate (BEC) by moving an optical dipole trap out of the condensate [6].

In this paper, we propose two concrete schemes to quickly extract thousands of neutral atoms from the Mott insulator (MI) state in optical lattices [7,8] and prepare them in the ground states of optical microtrap arrays with precisely one atom per trap. In practice, a perfect MI state with one atom per lattice site may be obtained with suitable experimental parameters, following proper purification processes [9]. In MI states, atoms are isolated from each other and occupy the ground states of each site, making it difficult to realize a low density MI in long-lattice-spacing (d) laser geometries [10] where the MI energy scales ($\sim d^{-2}$) fall below characteristic temperatures. On the other hand, the size of a microtrap ($\sim 2\ \mu\text{m}$) is much larger than the typical lattice spacing ($\sim 0.4\ \mu\text{m}$), which makes it difficult to extract atoms to mi-

crotraps directly from a MI state. Therefore the main challenge, and also the goal of this paper, is to transfer single atoms from optical lattices with a *short* lattice period (SPOL) to spatially separate optical microtraps.

We show in the first scheme that such a transfer process may be accomplished using hyperfine-state-dependent optical lattices with a *long* lattice period (LPOL), microwave radiation, and resonant “removing” lasers. A LPOL is created by intersecting two laser beams at a certain angle, as demonstrated in a recent experiment [10]. The LPOL induces position-dependent energy shifts of the hyperfine states of atoms, which, when combined with microwave radiation and resonant “removing” lasers, expel many atoms out of the optical lattice and form a patterned loaded optical lattice with one atom per n lattice sites ($n \geq 3$ is an integer). The remaining atoms in the lattices are well separated and can be adiabatically transferred to the ground states of optical microtrap arrays with one atom per trap. With our scheme, thousands of atoms may be extracted and the failure probability in extraction can be kept below $\sim 10^{-4}$. In the second scheme, the transfer process is accomplished using state-dependent focused lasers without expelling atoms out of the optical lattice; therefore, more atoms can be extracted but the failure probability is much higher. These complementary schemes—one with very high fidelity (but relatively lower speed) and the other with very fast speed (but relatively lower fidelity)—take advantage of the robust localization inherent in the MI to isolate atoms.

The first extraction scheme includes four operational steps, and their time sequences are schematically plotted in Fig. 1(a). For simplicity, we focus on a one-dimensional (1D) geometry but we emphasize that our technique can be straightforwardly applied to two-dimensional arrays.

Step I: Initial Mott state. Consider a ^{87}Rb BEC prepared in the hyperfine ground state $|0\rangle \equiv |F=1, m_F=-1\rangle$ and confined in a quasi-one-dimensional (x direction) harmonic magnetic trap, with the frozen atomic dynamics along the transverse direction [11]. An optical lattice along the x direction with wavelength $\lambda_s=850\ \text{nm}$ is ramped up adiabatically ($\sim 200\ \text{ms}$) to a large potential depth of $V_s=50E_R$ such that the BEC is converted into a MI state [7]. Here $E_R = \hbar^2/2m\lambda_s^2$ denotes the recoil energy. This MI state may have defects [8], and clever purification schemes [9] may yield a

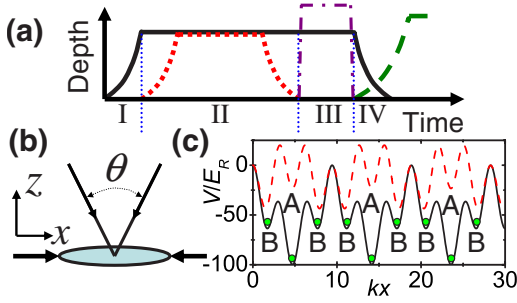


FIG. 1. (Color online) Schematic plot of the single atom extraction. (a) Time sequence for laser depths at four extraction steps. Solid line (SPOL), dotted line (LPOL), dash-dotted line (removing laser), and dashed line (microtrap laser). (b) Geometry of additional lasers defining the LPOL. (c) Site-specific energies in the optical lattice. Solid and dashed lines correspond to the optical potentials for atoms at states $|0\rangle$ and $|1\rangle$, respectively. A labels target atoms for extraction and B labels other atoms.

nearly perfect MI state with exact one atom per lattice site, which is the reservoir for single atom extraction and provides the starting point of our scheme.

Step II: Selective depopulation. Here atoms at specific, unwanted sites are transferred to another hyperfine state. Two σ^+ -polarized laser beams intersecting at an angle θ [Fig. 1(b)], which has a detuning $\Delta_2 = -2\pi \times 3608$ GHz to the $5^2P_{3/2}$ state (wavelength $\lambda_l = 787.6$ nm), are adiabatically ramped up. These two beams form a LPOL along the x direction with lattice period $\eta_l = \lambda_l / [2 \sin(\theta/2)]$. Here we require η_l to be n times $\lambda_s/2$, the period of the SPOL. The LPOL induces energy shifts

$$\delta E_{\pm}(r) = \frac{3\pi c^2 I(r)}{2} \sum_{q=1,2} \frac{\Gamma_q |c_{\pm q}|^2}{\omega_q^3 \Delta_q} \quad (1)$$

for two fine-structure ground states $|\pm\rangle = |5S; j=1/2, m_j = \pm 1/2\rangle$, where $I(r)$ is the intensity of the laser and Γ_q ($q=1,2$) is the decay rate for states $5^2P_{1/2}$ and $5^2P_{3/2}$. ω_q (Δ_q) is the frequency (detuning) for the transition from $5S$ to $5^2P_{1/2}$ and $5^2P_{3/2}$. $c_{\pm q}$ are transition coefficients. Two hyperfine states $|0\rangle$ and $|1\rangle = |F=2, m=-2\rangle$ can be written as $|0\rangle = 1/4|-\rangle + 3/4|+\rangle$, $|1\rangle = |-\rangle$ using the respective Clebsch-Gordan coefficients. Therefore the energy shifts for states $|0\rangle$ and $|1\rangle$ are $\delta E_0 = \delta E_-/4 + 3\delta E_+/4$ and $\delta E_1 = \delta E_-$, which give the total shift of the hyperfine splitting between $|0\rangle$ and $|1\rangle$, $\delta E = \delta E_1 - \delta E_0 = \alpha_1/2\Delta_1 - \alpha_2/2\Delta_2$, where $\alpha_q = 3\pi c^2 \Gamma_q I/2\omega_q^3$. Following a similar procedure, we find that the spontaneous emission rates for atoms at $|0\rangle$ and $|1\rangle$ are $\gamma_0 = \alpha_1 \Gamma_1/6\Delta_1^2 + 5\alpha_2 \Gamma_2/6\Delta_2^2$ and $\gamma_1 = 2\alpha_1 \Gamma_1/3\Delta_1^2 + \alpha_2 \Gamma_2/3\Delta_2^2$. Note that the detuning $\Delta_2 = -2\pi \times 3608$ GHz is optimized to obtain the maximal ratio $\eta = \delta E/\gamma$ between the shift δE and the rate $\gamma = \max\{\gamma_0, \gamma_1\}$.

In Fig. 1(c), we plot the combined lattice potentials for atoms at $|0\rangle$ and $|1\rangle$ with $n=3$. We see that the LPOL induces two different shifts of the hyperfine splitting, depending on the positions of atoms (A or B), and the difference $\delta = \delta E(A) - \delta E(B)$ can be adjusted and chosen to be $\delta = 52E_R$. Applying the adiabatic condition, we estimate the ramp-up

time to be $44 \mu\text{s}$, which corresponds to a 10^{-4} probability for excitation to higher bands.

We then apply a microwave π pulse to flip the quantum states of atoms at position B [Fig. 1(c)] from $|0\rangle$ to $|1\rangle$. The microwave is resonant with the hyperfine splitting of atoms at B, but has a detuning δ for atoms at A. A microwave frequency $\Omega(t) = \Omega_0 \exp(-\omega_0^2 t^2) (-t_f \leq t \leq t_f)$ is used to perform the π pulse. For parameters $\omega_0 = \delta/4 = 13E_R/\hbar$, $t_f = 5/\omega_0$, and $\Omega_0 = \pi / [\int_{-t_f}^{t_f} \exp(-\omega_0^2 t^2) dt] \approx 23E_R/\hbar$, the pulse flips the quantum state of atom B from $|0\rangle$ to $|1\rangle$ in $2t_f = 38.6 \mu\text{s}$, while the error to flip atom A to state $|1\rangle$ is found to be 5.9×10^{-6} by numerically integrating the Rabi equation [12] that describes the coupling between $|0\rangle$ and $|1\rangle$ through the microwave pulse. The LPOL are adiabatically turned off after the microwave pulse. During the whole process time τ , the probability for spontaneous scattering of one photon from each atom is estimated to be $P = \int_0^\tau \gamma dt \approx 1 \times 10^{-4}$.

Step III: Remove nontarget atoms. Atoms at B are removed from the trap by applying a “removing” laser that drives a resonant cycling transition $|1\rangle \rightarrow |2\rangle = |5^2P_{3/2}; F=3, m_F=-3\rangle$. Scattering photons from the laser push (or heat) nontarget atoms B at $|1\rangle$ out of the trap without affecting target atoms A at state $|0\rangle$ because of the large hyperfine splitting ($\nu \approx 2\pi \times 6.8$ GHz) between the two states. To push one nontarget atom out of a trap with depth U_0 , the number of spontaneous scattering photons needs to be at least $n_p = U_0/2E_R$ [4] (for example, 25 photons are needed for $U_0 = 50E_R$). n_p for both target and nontarget atoms can be calculated by numerically solving the optical Bloch equation [12]. We find that n_p can reach 25 in a short period $\sim 1 \mu\text{s}$ for atoms B, but it is only $\sim 10^{-5}$ for atoms A. Therefore the impact of the resonant laser on the target atoms A can be neglected. Note that hot nontarget atoms tunnel more easily in the optical lattice, which enhances the collision probability between target and nontarget atoms at different lattice sites. However, because of the high lattice depths ($\sim 50E_R$), the tunneling rate is quite low ($\sim 0.01E_R$) on average for hot nontarget atoms, which yields a long tunneling time (~ 100 ms). The short lifetime ($\sim 1 \mu\text{s}$) of hot nontarget atoms makes the collision probability very small ($\sim 1 \mu\text{s}/100 \text{ ms} = 10^{-5}$). The effect of interatomic collisions on the target atoms can therefore be neglected.

Step IV: Transfer to microtraps. The remaining target atoms A at the optical lattice are adiabatically distributed to the ground state of optical microtrap arrays with one atom per trap. Each optical microtrap is focused near one target atom and contains only one atom because of the large spacing between atoms. In the distribution process, the effective potentials the target atoms experience may be approximated as harmonic potentials with the trapping frequency $\omega(t) = \sqrt{[4V_f(t)/w^2 + 2V_L(t)k^2]}/m$, where $V_f(t)$ and $V_L(t)$ are the potential depths of the microtraps and the optical lattice, respectively, and w is the beam waist of the microtrap lasers. $V_f(t)$ and $V_L(t)$ may be varied simultaneously to adjust $\omega(t)$ from its initial value $\omega(0)$ to the final expected $\omega(t_0)$. If $\omega(t_0) = \omega(0)$, the final microtrap potential depth $V_f(t_0) \approx 1366E_R$ for initial parameters $V_L(0) = 50E_R$ and $w = 1 \mu\text{m}$.

When a deeper or shallower microtrap potential depth is needed, the trapping frequency $\omega(t)$ should be adjusted so that the adiabatic condition is satisfied:

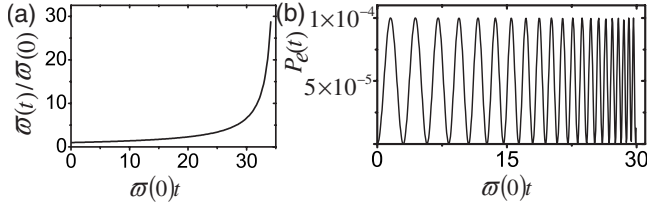


FIG. 2. (a) Plot of the trapping frequency $\varpi(t)$ with respect to time. (b) The probability $P_e(t) = |c_e|^2$ versus time.

$$\hbar |d\varpi(t)/dt| = \xi(\Delta E_g)^2 / \langle \phi_e | \partial H / \partial \varpi | \phi_g \rangle, \quad (2)$$

where $|\phi_g\rangle$ and $|\phi_e\rangle$ are the ground- and excited-state wave functions, ΔE_g is the energy gap between two states, and ξ is the adiabaticity parameter. Because of the parity of the wave functions, the lowest possible excitation is to the second excited state, which gives $\Delta E_g = 2\hbar\varpi$ and $\langle \phi_e | \partial H / \partial \varpi | \phi_g \rangle = \hbar/\sqrt{2}$. Equation (2) yields $\varpi(t) = \varpi(0) / [1 \mp 4\sqrt{2}\xi\varpi(0)t]$, where $-$ and $+$ correspond to a deeper and shallower final trapping frequency, respectively. Under the adiabatic approximation, the quantum states of the target atoms can be expanded using the time-dependent basis $\varphi(t) = c_g(t)\phi_g[\varpi(t)] + c_e(t)\phi_e[\varpi(t)]$, where $\phi_g[\varpi(t)]$, and $\phi_e[\varpi(t)]$ are the adiabatic ground and second excited states of the Hamiltonian $H[\varpi(t)]$ with the associated eigenenergies $E_g = \hbar\varpi(t)/2$ and $E_e = 5\hbar\varpi(t)/2$. Inserting this expansion into the Schrödinger equation for a single target atom A yields a coupled equation for the coefficients $c_g(t)$ and $c_e(t)$:

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_g \\ c_e \end{pmatrix} = \begin{pmatrix} E_g & \kappa(t) \\ -\kappa(t) & E_e \end{pmatrix} \begin{pmatrix} c_g \\ c_e \end{pmatrix}, \quad (3)$$

where $\kappa(t) = -i\hbar\dot{\varpi}(t)\langle \phi_e | \partial H / \partial \varpi | \phi_g \rangle / \Delta E_g = i\xi\Delta E_g$. This equation can be solved analytically to give the occupation probability at the second excited states, $P_e(t) = 4\xi^2 \sin^2[\ln(1 \mp 4\sqrt{2}\xi\varpi(0)t) / 4\sqrt{2}\xi]$.

In Fig. 2, we plot the trapping frequency $\varpi(t)$ and excitation probability $P_e(t)$ with respect to time for a deeper final trap. We see $P_e(t)$ has the maximum $4\xi^2$, which is 10^{-4} for $\xi = 0.005$. The total distribution time is $T = [1 - \varpi(0)/\varpi(T)] / [4\sqrt{2}\xi\varpi(0)]$. For instance, $T \approx 94 \mu\text{s}$ is needed to transfer target atoms from the optical lattice to microtraps with trapping frequency $\varpi(T) = 4\varpi(0)$ with 10^{-4} excitation probability. We note that this transfer time is much shorter than the characteristic hopping time (~ 5 s for $V_s = 50E_R$) of atoms within the depleted optical lattice.

Combining all four operational steps, we find that thousands of atoms can be extracted from the optical lattice to microtraps in less than $300 \mu\text{s}$. For instance, in a one-dimensional optical lattice with 300 usable atoms for single-atom extraction, we can extract 100 atoms. In a two-dimensional trap, the same process can extract 1/9 of total atoms ($\sim 10^4$) simultaneously, which offers a large scale-up in the initialization stage of a quantum computation using microtrap arrays.

The failure probability of extraction does not decrease with an increasing n , because the micro trap potential is very

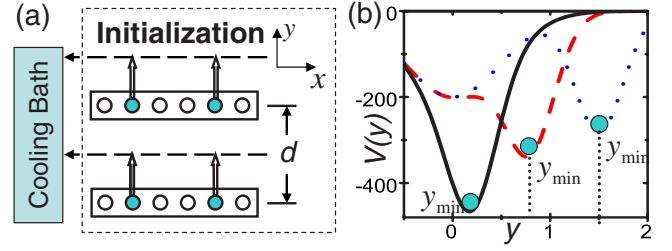


FIG. 3. (Color online) (a) Schematic plot for the single-atom extraction from parallel one-dimensional lattices. The distance $d = 5 \mu\text{m}$. Solid and open circles correspond to target and nontarget atoms, respectively. (b) Optical potentials for target atoms along the y direction. The length and energy units are σ_c and $\hbar^2/2m\sigma_c^2$, respectively. $a(t) = 0.2\sigma_c$ (solid line), $a(t) = 0.8\sigma_c$ (dashed line), and $a(t) = 1.5\sigma_c$ (dotted line).

weak at $a \sim 1.3 \mu\text{m}$ displacement (positions of neighboring atoms in a $n=3$ superlattice) from the trap center for a typical $\sim 2 \mu\text{m}$ microtrap. The potential has a negligible effect on the process of transferring neighboring atoms to other microtraps. A large- n lattice does not contribute to the largest error source of the scheme: the heating due to spontaneously scattered photons from atoms in the state-dependent lattice in step II.

Speedup scheme. In the above scheme, the qubit supply time for quantum computation is limited by the period for preparing Bose-Einstein condensates, which is typically on the order of minutes. Note that in step III most atoms are lost from the lattice. In the following, we propose a scheme without removing nontarget atoms, which can then be recycled for further extraction processes. In this scheme, 87% of the atoms can be extracted within several superfluid-insulator transition cycles (~ 1 s), considerably speeding up the rate for supplying fresh qubits for a neutral-atom quantum computer. However, the scheme induces much larger heating of the target atoms, which significantly degrades the fidelity of the initial qubit; therefore, further cooling is needed to obtain qubits with high fidelity.

A schematic for the speedup scheme is plotted in Fig. 3(a). Consider a series of parallel well-separated ($d = 5 \mu\text{m}$) 1D optical lattices (along the x direction) in the xy plane. In the speedup scheme, steps I and II are still performed to place all target atoms for extraction into state $|0\rangle$ and nontarget atoms to $|1\rangle$. We then ramp up properly chosen focused lasers which induce red-detuned traps for target atoms at state $|0\rangle$, but do not affect nontarget atoms at state $|1\rangle$ [13]. The focused lasers adiabatically move along the y direction to take target atoms out of the optical lattices, without affecting nontarget atoms at state $|1\rangle$ [Fig. 3(a)]. The atoms inside the focused lasers are then adiabatically transferred to far-detuned dipole traps to suppress spontaneous emission of photons. These dipole traps are moved along the x direction to a cooling bath to improve the fidelity of the initial qubits. At the same time, the Mott insulator states in the optical lattices are melted by adiabatically ramping down the depth of the optical lattice. The trap parameters are adjusted so that another Mott state with one atom per lattice site can be obtained as the lattice depths are adiabatically ramped up. Repeating the above steps, we can extract another 1/3 of the

remaining atoms. After 5 such cycles, about $1-(2/3)^5 \approx 87\%$ atoms can be extracted. Finally, the remaining atoms inside the optical lattices are discarded and a new BEC must be produced to continue the process.

To extract the atoms adiabatically from optical lattices avoiding excitations to higher bands of the focused laser traps, high potential depths are needed, which leads to high spontaneous photon scattering probabilities. Therefore a good strategy balances these two sources for the degradation of initial qubit fidelity. Assume that the optical potentials along the y direction for target atoms are

$$V(y) = -V_c \exp(-2y^2/\sigma_c^2) - V_f \exp\{-2[y - a(t)]^2/\sigma_f^2\}, \quad (4)$$

where V_c and V_f are the potential depths for the 1D confinement and the focused laser, respectively. Gaussian beam approximations with waists σ_c and σ_f have been used for a rough estimate. $a(t)$ is the position of the focused laser center, and its rate of change should satisfy the adiabatic condition $\hbar|da(t)/dt| = \bar{\xi} \Delta E_g^2 / |\langle \phi_e | \partial H / \partial a | \phi_g \rangle|$, where the energy gap ΔE_g and transition matrix element $|\langle \phi_e | \partial H / \partial a | \phi_g \rangle|$ can be evaluated for different potentials $V(a(t))$ by solving the single-particle Schrödinger equation. The potential minimum position y_{\min} for the target atom is determined through $\partial V / \partial y = 0$. The wave function of the target atom is expanded in a harmonic oscillator basis $\Psi_n(y) = (\kappa/\pi)^{1/4} \exp[-\kappa(y - y_{\min})^2/2] H_n(\sqrt{\kappa}y) / \sqrt{2^n n!}$ around the potential minimum y_{\min} , where the oscillation frequency $\kappa = (\partial^2 V / \partial y^2)_y / m$

and $H_n(\sqrt{\kappa}y)$ is the Hermite polynomial. The Hamiltonian for the target atoms evaluated in this basis for different $a(t)$ gives the matrix representation $H_{nm}(a(t)) = \langle \Psi_n | H | \Psi_m \rangle$ ($n, m \leq 10$ is enough for our calculation). Diagonalization of the matrix yields the eigenenergies and eigenfunctions, which determine ΔE_g and $|\langle \phi_e | \partial H / \partial a | \phi_g \rangle|$ for different $a(t)$. The total moving time can be estimated using

$$T = \int_0^{a_f} \hbar |\langle \phi_e | \partial H / \partial a | \phi_g \rangle| / \bar{\xi} \Delta E_g^2 da, \quad (5)$$

where a_f is the final position of the focused laser.

In Fig. 3(b), we plot the optical potential $V(y)$ for a set of parameters $\sigma_c \approx 0.93 \mu\text{m}$, $\sigma_f \approx 0.46 \mu\text{m}$, $V_c = 200\hbar^2/m\sigma_c^2$, $V_f = 280\hbar^2/m\sigma_c^2$, and three different $a(t)$. Applying the above procedure with these parameters, we estimate the extraction time ~ 5 ms and the excitation probability to high bands, $\sim 7 \times 10^{-3}$, with the spontaneous scattering probability $\sim 10^{-2}$. We see that the fidelity of the atoms is not as high as that for the original scheme. Therefore further cooling is needed to significantly improve the fidelity of initial qubits.

Conclusion. We propose two schemes for extracting thousands of atoms simultaneously from the Mott-insulator state in optical lattices to optical microtrap arrays with one atom per trap. The extracted atoms stay at the ground states of the microtraps. We provide a detailed quantitative analysis validating the feasibility of our proposed schemes for neutral-atom quantum computation.

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