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Atom number filter in an optical lattice

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Abstract. We present an efficient procedure to filter out from an optical lattice, having inhomogeneous site occupation number, only preselected number of bosonic atoms per site and place them into another internal atomic state, creating thereby a lattice with desired site occupation number.

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‡ This paper is dedicated to Peter Lambropoulos on the occasion of his 75 year jubilee.

Ultracold atoms in optical lattices [1] represent a remarkably clean and controllable system [2, 3] to realize the fundamental Bose-Hubbard model [4]. Its two main ingredients are the atom tunneling, or hopping J , between the neighbouring lattice sites and the on-site atom-atom interaction U . In a homogeneous lattice, when the kinetic energy due to the inter-site hopping dominates, $J \gtrsim U$, the atoms are delocalized over the entire lattice yielding a superfluid (SF) phase, while in the opposite regime of strong on-site interaction, $U \gg J$, the hopping is energetically suppressed resulting in a Mott insulator (MI) phase with fixed integer number n of localized atoms at each lattice site. When a deep optical lattice is superimposed by a shallow confining potential, there can be MI phases with occupation numbers of $n = 0, 1, 2, \dots$ in successive spatial shells [5, 6, 7, 8], separated by SF phases with intermediate mean occupation number corresponding to delocalized atoms on top of the filled MI shell.

Experimentally [3], the quantum phase transition between the SF and MI phases is implemented by adiabatically increasing the lattice depth which results in the reduction of intersite tunneling amplitude and simultaneous increase of the on-site interaction [2]. If, however, the lattice potential is raised quickly, so that the tunneling is suddenly switched off, each site occupation “freezes” to whatever atom-number distribution it corresponded to just before the switching off, be it a SF, a MI, or a spatially-dependent combination of the two phases.

In this paper, we propose a very efficient method to filter out from such a frozen ($J = 0$) optical lattice only the desired number N of atoms per site. This is achieved by using an external field which couples the initially populated internal atomic state $|a\rangle$ to another internal state $|b\rangle$ trapped by a second optical lattice potential. We show that, for strong enough state- (or lattice-) dependent on-site interactions, the coupling field with properly tuned frequency will selectively transfer to the second lattice only the singles ($N = 1$), the pairs ($N = 2$), or the triples ($N = 3$) of atoms, via the corresponding N -photon resonant transition. Hence, after the transfer, the second lattice will only have the desired site occupation number $N = 1, 2$, or 3 , while the first lattice will contain all the other occupation numbers $n \neq N$.

Before proceeding, we note related, but different, earlier work. Rabl *et al* [9] proposed to reduce the site occupation number defects in an optical lattice by adiabatically transferring a chosen number of atoms to another internal state. DeMarco *et al* [5] studied similar systems employing rapid adiabatic transfer of atoms to the second internal state, or inducing resonant single-photon Rabi oscillations between the atomic states with occupation number-dependent Rabi frequencies. Mohring *et al* [10] discussed coherent extraction of atoms from a BEC reservoir into the quantum tweezers—tight trap—using adiabatic and resonant transfer techniques. del Campo *et al* [11] described the preparation of number states of strongly interacting atoms by reducing the depth and width of a one-dimensional trap.

Considering only two internal atomic states and corresponding optical lattice

potentials, the Hamiltonian of the system takes the form

$$\begin{aligned}
H = \sum_j & [(\hbar\omega_a + \varepsilon_{a,j})\hat{n}_{a,j} + \frac{1}{2}U_{aa}\hat{n}_{a,j}(\hat{n}_{a,j} - 1) \\
& + (\hbar\omega_b + \varepsilon_{b,j})\hat{n}_{b,j} + \frac{1}{2}U_{bb}\hat{n}_{b,j}(\hat{n}_{b,j} - 1) \\
& + U_{ab}\hat{n}_{a,j}\hat{n}_{b,j} + \hbar\Omega(\hat{b}_j^\dagger\hat{a}_j e^{-i\omega t} + \hat{a}_j^\dagger\hat{b}_j e^{i\omega t})].
\end{aligned} \tag{1}$$

Here \hat{a}_j (\hat{a}_j^\dagger) and \hat{b}_j (\hat{b}_j^\dagger) are the annihilation (creation) operators for bosonic atoms in the internal states $|a\rangle$ and $|b\rangle$, of energies $\hbar\omega_a$ and $\hbar\omega_b$, localized at lattice site j , with single-particle energies $\varepsilon_{a,j}$ and $\varepsilon_{b,j}$, and $\hat{n}_{a,j} \equiv \hat{a}_j^\dagger\hat{a}_j$ and $\hat{n}_{b,j} \equiv \hat{b}_j^\dagger\hat{b}_j$ are the corresponding number operators. A natural basis for Hamiltonian (1) is that of the eigenstates $|n_{\alpha,j}\rangle$ of operators $\hat{n}_{\alpha,j}$ whose eigenvalues $n = 0, 1, 2, \dots$ denote the number of atoms in the corresponding state $|\alpha\rangle$ ($\alpha = a, b$) at site j . Next, $U_{\alpha\alpha} = g_{\alpha\alpha} \int d^3r |w_\alpha(\mathbf{r})|^4$ is the on-site interaction energy for the atoms in state $|\alpha\rangle$, and $U_{ab} = g_{ab} \int d^3r |w_a(\mathbf{r})|^2 |w_b(\mathbf{r})|^2$ is the interaction between the $|a\rangle$ and $|b\rangle$ atoms, where $g_{\alpha\alpha'} \equiv 4\pi a_{\alpha\alpha'} \hbar^2/M$, with $a_{\alpha\alpha'}$ being the corresponding s -wave scattering length, M the atomic mass and $w_\alpha(\mathbf{r})$ the (localized) Wannier function of the lowest Bloch band of the corresponding lattice potential [1, 2]. Finally, $\Omega = \Omega_{ab} \int d^3r w_a^*(\mathbf{r})w_b(\mathbf{r})$ is the coupling amplitude between the localized atoms in states $|a\rangle$ and $|b\rangle$, which is induced by an external field with the “bare” (free-atom) Rabi frequency Ω_{ab} . This field can be a microwave field of frequency $\omega \sim \omega_b - \omega_a$ coupling the atomic hyperfine states $|a\rangle$ and $|b\rangle$ through a magnetic dipole transition, or an optical bi-chromatic field inducing Raman transition $|a\rangle \rightarrow |b\rangle$, in which case ω is the frequency difference between the two field components (the corresponding differential ac Stark shift of $|a\rangle$ and $|b\rangle$ can be incorporated in ω_a or ω_b). Note that the rotating-wave approximation, requiring $\Omega \ll \omega$, is presumed in the last term of equation (1).

In deep optical lattices, the Wannier functions $w_\alpha(\mathbf{r} - \mathbf{r}_{\alpha,j})$ localized on individual sites j can be well approximated [1] by the ground-state wavefunction of a harmonic oscillator centered at $\mathbf{r}_{\alpha,j}$,

$$w_\alpha(\mathbf{r} - \mathbf{r}_{\alpha,j}) \approx \left(\frac{1}{\pi\sigma_\alpha^2}\right)^{3/4} \exp\left[-\frac{(\mathbf{r} - \mathbf{r}_{\alpha,j})^2}{2\sigma_\alpha^2}\right], \tag{2}$$

where the width $\sigma_\alpha = \sqrt{\hbar/M\nu_\alpha}$ is expressed through the vibrational frequency $\nu_\alpha = \sqrt{2\pi^2 V_\alpha/Md^2}$ determined by the lattice potential amplitude V_α and period d . For the interaction parameters of Hamiltonian (1) we then obtain

$$U_{\alpha\alpha} \simeq \frac{g_{\alpha\alpha}}{(2\pi\sigma_\alpha^2)^{3/2}} \propto a_{\alpha\alpha} V_\alpha^{3/4} \quad (\alpha = a, b), \tag{3a}$$

$$U_{ab} \simeq \frac{g_{ab}}{[\pi(\sigma_a^2 + \sigma_b^2)]^{3/2}} \exp\left[-\frac{\delta r^2}{\sigma_a^2 + \sigma_b^2}\right], \tag{3b}$$

$$\Omega \simeq \Omega_{ab} \left(\frac{\sigma_a\sigma_b}{\sigma_a^2 + \sigma_b^2}\right)^{3/2} \exp\left[-\frac{\delta r^2}{2(\sigma_a^2 + \sigma_b^2)}\right], \tag{3c}$$

where $\delta r \equiv |\mathbf{r}_{a,j} - \mathbf{r}_{b,j}| < d$ is a possible offset of the lattice potentials for the atoms in states $|a\rangle$ and $|b\rangle$ [12]. These expressions attest to the controllability of the atom-

atom interactions $U_{\alpha\alpha'}$ and coupling Ω through the interatomic scattering lengths $a_{\alpha\alpha'}$ ($\alpha, \alpha' = a, b$); the optical lattice parameters, including the lattice modulation depths V_α , affecting σ_α 's, and the relative offset δr ; as well as the external coupling field amplitude, affecting Ω_{ab} . In the experiments, typically $U_{\alpha\alpha'}/\hbar \lesssim 2\pi \times 10$ kHz [1, 3, 6, 7]. We emphasise that the single-band approximation inherent in Hamiltonian (1) requires that the atom-atom interactions be small compared to the excited band energies, $U_{\alpha\alpha'} < \hbar\nu_\alpha$.

While, in general, $\varepsilon_{a,j}$ and $\varepsilon_{b,j}$ need not be uniform throughout the lattice, due to, e.g., shallow external trap, we assume that the difference $|\varepsilon_{a,j} - \varepsilon_{b,j}|$ is constant, and typically small compared to $\omega_b - \omega_a$, for all j . Accordingly, we define $\hbar\omega_{ba} \equiv \hbar\omega_b + \varepsilon_{b,j} - (\hbar\omega_a + \varepsilon_{a,j}) = \text{const} \forall j$ and omit the subscript j from now on.

Assume that initially all the atoms are in state $|a\rangle$, with the sites of the corresponding lattice having arbitrary occupations $|n_a\rangle$, $n = 0, 1, 2, \dots$, and all the sites of the other lattice empty, $|0_b\rangle$.

Before describing our main idea of atom-number filter, we briefly consider a simple but instructive case of uniformly interacting $U_{\alpha\alpha'} = U$ ($\alpha, \alpha' = a, b$), or non-interacting $U = 0$, atoms subject to a resonant coupling field $\omega = \omega_{ba}$. Within an N -atom subspace ($N = n_a + n_b = \text{const}$), the transition matrix element of Hamiltonian (1) between any pair of states of the form $|(N - n)_a, n_b\rangle$ and $|(N - n - 1)_a, (n + 1)_b\rangle$ is given by $\hbar\Omega\sqrt{(N - n)(n + 1)}$, as dictated by the bosonic nature of the atoms. This system is formally analogous to a spin- \mathcal{J} in a transverse magnetic field. Indeed, defining the operators $\hat{J}_x = \frac{1}{2}(\hat{b}^\dagger\hat{a} + \hat{a}^\dagger\hat{b})$, $\hat{J}_y = -\frac{i}{2}(\hat{b}^\dagger\hat{a} - \hat{a}^\dagger\hat{b})$ and $\hat{J}_z = \frac{1}{2}(\hat{b}^\dagger\hat{b} - \hat{a}^\dagger\hat{a})$ which obey the standard angular momentum commutation relations, the Hamiltonian (1) at a single lattice site can be written as a spin Hamiltonian $H_{\text{spin}} = 2\hbar\Omega\hat{J}_x$, to within constant energy $\frac{1}{2}UN(N - 1)$. The matrix elements of H_{spin} for the transitions $|\mathcal{J}, m\rangle \rightarrow |\mathcal{J}, m + 1\rangle$ between the neighboring magnetic sub-states ($m = -\mathcal{J}, \dots, \mathcal{J}$) are given by $\hbar\Omega\sqrt{(\mathcal{J} - m)(\mathcal{J} + m + 1)}$, which result in non-dispersive precession of the spin about the field direction with the Larmor frequency Ω being independent of \mathcal{J} . Setting formally $\mathcal{J} = \frac{1}{2}N$ and $m = n - \frac{1}{2}N$ leads to the above matrix elements of (1). A curious consequence of this analogy is that, within *any* N -atom subspace, the resonant coupling field will induce oscillations between states $|N_a, 0_b\rangle$ and $|0_a, N_b\rangle$ with the *same* frequency Ω . And in particular, starting from all the atoms in state $|a\rangle$ and arbitrary site occupation numbers of the corresponding lattice, at time $\tau = \pi/2\Omega$, all the atoms will simultaneously be transferred to state $|b\rangle$.

We now discuss the transfer of selected number of atoms N between the two lattices, as illustrated in figure 1 (left panel). This atom-number filtering procedure is very simple yet remarkably efficient and robust, provided

$$|U_{ab} - \frac{1}{2}(U_{aa} + U_{bb})| \gg \hbar\Omega, \quad (4a)$$

$$|U_{aa} - U_{bb}|, |U_{ab} - U_{aa,bb}| \gg \hbar\Omega. \quad (4b)$$

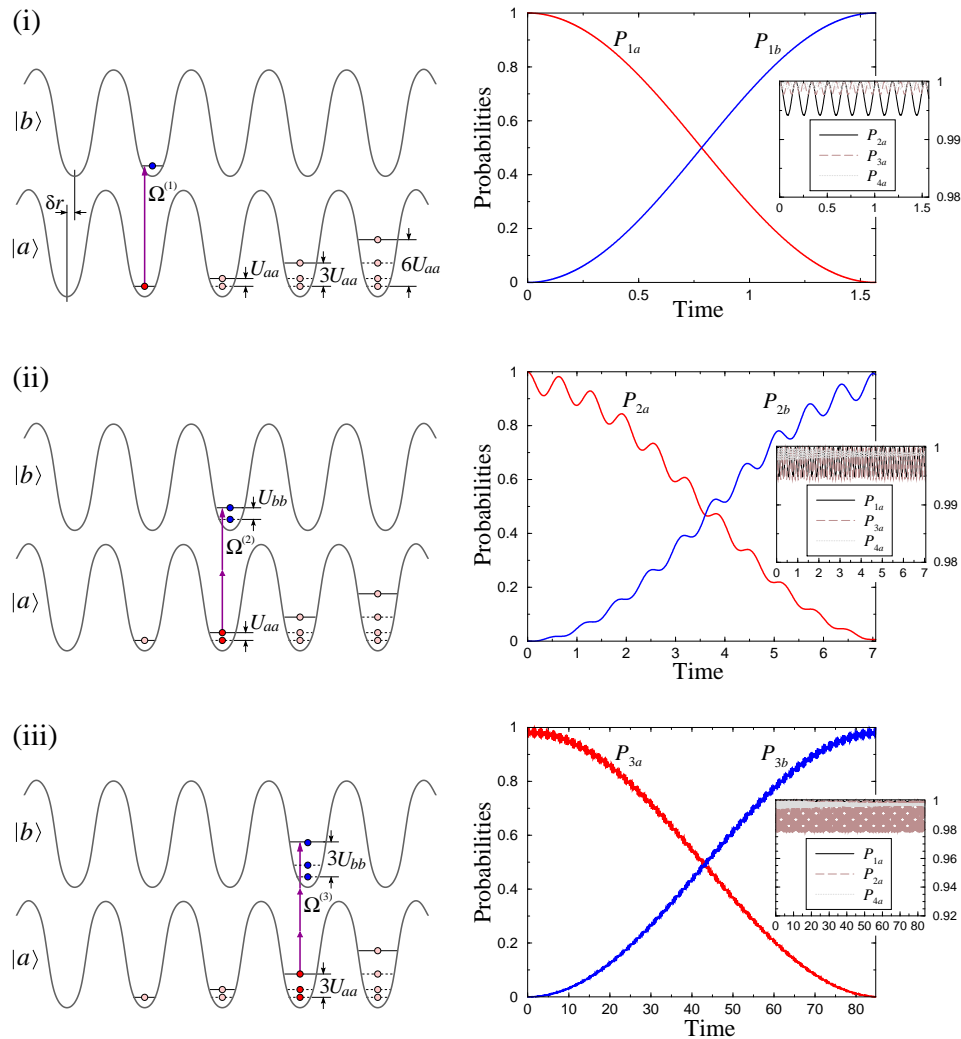


Figure 1. Schematics (left column) and dynamics (right column) of atom transfer between two optical lattices: selective transfer of (i) single atoms, $N = 1$; (ii) pairs of atoms, $N = 2$; and (iii) triples of atoms, $N = 3$, via the corresponding N -photon resonant transitions. The main graphs display the probabilities $P_{N\alpha}$ for N atoms in the corresponding states $|\alpha\rangle$ ($\alpha = a, b$), while the insets show the probabilities $P_{n\alpha}$ of initial states $|n_a\rangle$ with $n \neq N$. (For $n > 4$, the probabilities $P_{n\alpha}$ oscillate with even smaller amplitudes and therefore not shown.) The numerical simulations employ the parameters $U_{\alpha\alpha'}$ and Ω listed in the text, the time is in units of Ω^{-1} and the evolution terminates at the corresponding $\tau^{(N)}$.

The first of these conditions ensures that within the selected N -atom subspace all the intermediate states are nonresonant, while the remaining conditions are needed to suppress all the transitions out of the other initial states $|n_a\rangle$ with $n \neq N$, as clarified below. For convenience we denote $\delta U \equiv [U_{ab} - \frac{1}{2}(U_{aa} + U_{bb})]/\hbar$.

(i) *Single atom transfer, $N = 1$.* To filter out only the single atoms per site, we tune the frequency of the coupling field to be resonant with the atomic transition $|a\rangle \rightarrow |b\rangle$, i.e., we set $\omega = \omega_{ba}$. The field will then induce resonant Rabi oscillations between

the states $|1_a, 0_b\rangle$ and $|0_a, 1_b\rangle$ with frequency $\Omega^{(1)} = \Omega$. If we apply the field for time $\tau^{(1)} = \pi/2\Omega^{(1)}$, resulting in a π -pulse, all the single atoms $|1_a\rangle$ will be transferred to $|1_b\rangle$.

(ii) *Two atom transfer, $N = 2$.* To filter out only the pairs of atoms per site, we choose the frequency of the coupling field according to the condition $2\omega = 2\omega_{ba} + (U_{bb} - U_{aa})/\hbar$, which implies a two-atom (and two-photon) transition $|2_a, 0_b\rangle \rightarrow |1_a, 1_b\rangle \rightarrow |0_a, 2_b\rangle$ via nonresonant intermediate state $|1_a, 1_b\rangle$ detuned by δU . The corresponding two-atom (-photon) Rabi frequency is then $\Omega^{(2)} = 2\Omega^2/\delta U$ (the factor of $2 = 2!$ originates from double application of bosonic operators $\hat{b}^\dagger\hat{a}$ to the initial state $|2_a, 0_b\rangle$), and at time $\tau^{(2)} = \pi/2\Omega^{(2)}$, corresponding to an effective π -pulse, all the pairs of atoms $|2_a\rangle$ will be transferred to $|2_b\rangle$.

(iii) *Three atom transfer, $N = 3$.* To filter out only the triples of atoms per site, we choose the frequency of the coupling field according to the condition $3\omega = 3\omega_{ba} + 3(U_{bb} - U_{aa})/\hbar$, which implies a three-atom (-photon) transition $|3_a, 0_b\rangle \rightarrow |2_a, 1_b\rangle \rightarrow |1_a, 2_b\rangle \rightarrow |0_a, 3_b\rangle$ via nonresonant intermediate states $|2_a, 1_b\rangle$ and $|1_a, 2_b\rangle$ both detuned by the equal amount of $2\delta U$. The corresponding three-atom (-photon) Rabi frequency is then $\Omega^{(3)} = 6\Omega^3/(2\delta U)^2$ (the factor of $6 = 3!$ originates from triple application of $\hat{b}^\dagger\hat{a}$ to state $|3_a, 0_b\rangle$). Note that since both intermediate states $|2_a, 1_b\rangle$ and $|1_a, 2_b\rangle$ have the same detuning $2\delta U$, the second-order ac Stark shifts of states $|3_a, 0_b\rangle$ and $|0_a, 3_b\rangle$ are the same, given by $3\Omega^2/(2\delta U)$, and the differential shift on the three-photon transition $|3_a, 0_b\rangle \rightarrow |0_a, 3_b\rangle$ vanishes. Hence, applying the field for time $\tau^{(3)} = \pi/2\Omega^{(3)}$, corresponding to an effective π -pulse, all the triples of atoms $|3_a\rangle$ will be transferred to $|3_b\rangle$.

The above procedure can be generalized to multiphoton transfer of any number of atoms N between the two lattices. Under the N -photon resonance condition $N\omega = N\omega_{ba} + \frac{1}{2}N(N-1)(U_{bb} - U_{aa})/\hbar$, the effective N -atom (-photon) Rabi frequency is then given by

$$\Omega^{(N)} = \frac{N!\Omega^N}{[(N-1)!]^2\delta U^{N-1}} = \frac{N\Omega}{(N-1)!} \left(\frac{\Omega}{\delta U}\right)^{N-1}.$$

However, due to the above scaling of $\Omega^{(N)}$ and condition $\Omega \ll |\delta U|$, the corresponding transfer time $\tau^{(N)} = \pi/2\Omega^{(N)}$ will become prohibitively long for $N \geq 4$ in a realistic optical lattice experiment, as discussed below.

In figure 1 (right panel) we demonstrate, via numerical solution of the corresponding Schrödinger equations, that the transfer of the selected number of atoms $N = 1, 2$ and 3 between the two lattices is indeed very efficient, with the probabilities $P_{N_b}(\tau^{(N)})$ of the final states $|N_b\rangle$ at the corresponding times $\tau^{(N)}$ being close to unity, while the probabilities P_{n_a} of initial states $|n_a\rangle$ with $n \neq N$ changing very little during the transfer. For these simulations, we choose $U_{aa}/\hbar \simeq 2\pi \times 10^4 \text{ s}^{-1}$, and, upon assuming $a_{aa} \simeq a_{bb} \simeq a_{ab}$, $V_a/V_b = 3$ and $\delta r = 0$, obtain from equations (3) $U_{bb} \simeq 0.44U_{aa}$

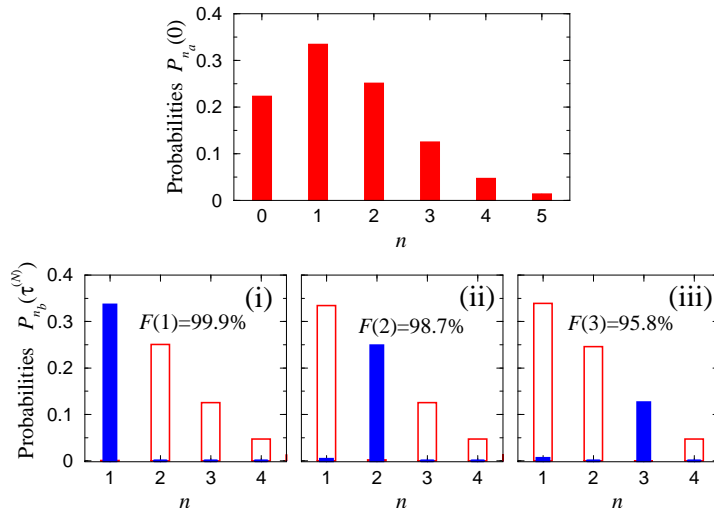


Figure 2. Filtering out of the initial Poisson distribution with mean atom number $\langle n \rangle_a = 1.5$ (top panel graph) single atoms (i), pairs of atoms (ii), and triples of atoms (iii). In the lower panel graphs, the empty (red) bars show the atom-number probability distributions $P_{n_a}(\tau^{(N)})$ remaining in the first lattice after the transfer. The transfer fidelities $F(N)$ are defined in equation (5). All parameters are as in figure 1.

and $U_{ab} \simeq 0.63U_{aa}$. We then have $\delta U \simeq 2\pi \times 930 \text{ s}^{-1}$ and set $\Omega = 2\pi \times 100 \text{ s}^{-1}$. The corresponding one-, two- and three-atom transfer times are given, respectively, by $\tau^{(1)} = 2.38 \times 10^{-3} \text{ s}$, $\tau^{(2)} = 1.16 \times 10^{-2} \text{ s}$ and $\tau^{(3)} = 0.144 \text{ s}$, which are shorter than the typical lifetimes (0.5 s) of cold atoms in optical lattice MI shells with $n \leq 3$ [6].

Hence, using our procedure one can separate the spatial MI shells of the optical lattice with different atom numbers n [6, 7], placing in another lattice only the desired N th shell, which can be a filled sphere (or circle in 2D), or a hollow sphere (ring in 2D), depending on whether it is extracted from the central part of the trap or not. This is then followed by discarding (releasing) the atoms of the first lattice. Another useful application of our atom-number filtering technique is a preparation of pure samples of the interaction-bound lattice dimers [13, 14, 15, 16], or trimers [17], without resorting to more complicated procedures involving Feshbach association, purification and dissociation of atom pairs [13, 18].

As an example, in figure 2 we illustrate the filtering out of the initial Poisson atom-number distribution $P_{n_a}(0) = \langle n \rangle^n e^{-\langle n \rangle} / n!$, corresponding to a frozen SF phase with mean occupation number $\langle n \rangle_a = 1.5$, the desired number of atoms $N = 1, 2$ or 3 . The only variables adjusted to each N case are the coupling field frequency ω and transfer time $\tau^{(N)}$, with all the other parameters the same, as described above in connection with figure 1. We quantify the transfer using the fidelity

$$F(N) = \frac{P_{N_b}(\tau^{(N)})}{\sum_{n>0} P_{n_b}(\tau^{(N)})}, \quad (5)$$

for which we obtain very high values $F(1) = 0.999$, $F(2) = 0.987$ and $F(3) = 0.958$.

To conclude, we have proposed and analysed a very efficient and robust procedure to filter out from an optical lattice with an arbitrary inhomogeneous site occupation number only preselected number of bosonic atoms per site and place them into another internal atomic state, creating thereby a lattice with desired site occupation number, which we envision to have a number of interesting applications.

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