FAST TRACK COMMUNICATION

Atom-number filter in an optical lattice

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Received 31 March 2010, in final form 29 April 2010
Published 17 June 2010
Online at stacks.iop.org/JPhysB/43/131001

Abstract

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

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 tunnelling, 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 a 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 $n = 0, 1, 2, \ldots$ in successive spatial shells [5–8], separated by SF phases with intermediate mean occupation numbers corresponding to delocalized atoms on top of the filled MI shells.

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 the inter-site tunnelling amplitude and simultaneous increase of the on-site interaction [2]. If, however, the lattice potential is raised quickly, so that the tunnelling is suddenly switched off, each site occupation ‘freezes’ to whatever atom-number distribution it corresponded to just before the switching off, be it an SF, an MI or a spatially dependent combination of the two phases.

In this communication, 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 the number states of strongly interacting atoms by reducing the depth and width of a one-dimensional trap.

* This paper is dedicated to Peter Lambropoulos on the occasion of his jubilee.

0953-4075/10/131001+05$30.00 © 2010 IOP Publishing Ltd Printed in the UK & the USA
Considering only two internal atomic states and corresponding optical lattice potentials, the Hamiltonian of the system takes the form

\[
H = \sum_j \left[ (\hbar \omega_a + \epsilon_{a,j}) \hat{n}_{a,j} + \frac{1}{2} U_{aa} \hat{n}_{a,j} (\hat{n}_{a,j} - 1) \right. \\
+ (\hbar \omega_b + \epsilon_{b,j}) \hat{n}_{b,j} + \frac{1}{2} U_{bb} \hat{n}_{b,j} (\hat{n}_{b,j} - 1) \\
+ U_{ab} \hat{n}_{a,j} \hat{n}_{b,j} + h \Omega (\hat{a}_j^\dagger \hat{a}_j e^{-i\omega t} + \hat{b}_j^\dagger \hat{b}_j e^{i\omega t}). \tag{1}
\]

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 the lattice site $j$, with single-particle energies $\epsilon_{a,j}$ and $\epsilon_{b,j}$, 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 $|n_{a,j}\rangle$ of operators $\hat{n}_{a,j}$ whose eigenvalues $n = 0, 1, 2, \ldots$ denote the number of atoms in the corresponding state $|a\rangle (a = a, b)$ at site $j$. Next, $U_{aa} = g_{aa} \int d^3 r |w_a(r)|^4$ is the on-site interaction energy for the atoms in the state $|a\rangle$ and $U_{ab} = g_{ab} \int d^3 r |w_a(r)| |w_b(r)|^2$ is the interaction between the $|a\rangle$ and $|b\rangle$ atoms, where $g_{aa} \equiv \pi \hbar \omega_a h^2 / M$, with $\omega_a$, being the corresponding s-wave scattering length, $M$ the atomic mass and $w_a(r)$ the (localized) Wannier function of the lowest Bloch band of the corresponding lattice potential [1, 2]. Finally, $\Omega = \Omega_{ab} \int d^3 r w_a(r) w_b(r)$ is the coupling amplitude between the localized atoms in the states $|a\rangle$ and $|b\rangle$, which is induced by an external field with the ‘bare’ (free-atom) Rabi frequency $\Omega_{ab}$. 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 the Raman transition $|a\rangle \rightarrow |b\rangle$, in which case $\omega$ 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 $\omega_a$ or $\omega_b$). 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 $w_a(r - r_{a,j})$ localized on the individual sites $j$ can be well approximated [1] by the ground-state wavefunction of a harmonic oscillator centred at $r_{a,j}$:

\[
w_a(r - r_{a,j}) \approx \frac{1}{(\pi \sigma_a^2)^{3/4}} \exp \left[ -\frac{\|r - r_{a,j}\|^2}{2\sigma_a^2} \right], \tag{2}
\]

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

\[
U_{aa} \simeq g_{aa} \left( \frac{2\pi \sigma_a^2}{\sqrt{\pi} \sigma_a^2} \right)^{3/2} \propto a_{a,j} V_a^{3/4} \quad (a = a, b), \tag{3a}
\]

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

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

where $\delta r \equiv |r_{a,j} - r_{b,j}| < d$ is a possible offset of the lattice potentials for the atoms in the states $|a\rangle$ and $|b\rangle$ [12]. These expressions attest to the controllability of the atom–atom interactions $U_{aa'}$ and coupling $\Omega$ through the interatomic scattering lengths $a_{aa'} (a, a' = a, b)$ and the optical lattice parameters, including the lattice modulation depths $V_a$, affecting $\sigma_a$, and the relative offset $\delta r$, as well as the external coupling field amplitude, affecting $\Omega_{ab}$. In the experiments, typically $U_{aa}/\hbar \lesssim 2\pi \times 10^5$ kHz [1, 3, 6, 7]. We emphasize that the single-band approximation inherent in Hamiltonian (1) requires that the atom–atom interactions be small compared to the excited band energies $U_{aa'} < \hbar V_a$.

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

Assume that initially all the atoms are in the state $|a\rangle$, with the sites of the corresponding lattice having arbitrary occupations $|n_{a,j}\rangle, n = 0, 1, 2, \ldots$, and all the sites of the other lattice empty, $|0_{b}\rangle$.

Before describing our main idea of the atom-number filter, we briefly consider a simple but instructive case of uniformly interacting $U_{aa} = U (\alpha \alpha', \alpha = a, b)$, or non-interacting $U = 0$, atoms subject to a resonant coupling field $\omega = \omega_b$. 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 $|N-n_{a,j}\rangle$ and $|(N-n_{b,j})\rangle$ 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-$J$ in a transverse magnetic field. Indeed, defining the operators $J_z = \frac{1}{2} (\hat{b}_j^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{b}_j)$, $J_y = -\frac{1}{\sqrt{2}} (\hat{b}_j^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{b}_j)$ and $J_x = \frac{1}{\sqrt{2}} (\hat{b}_j^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{b}_j)$ which obey the standard angular momentum commutation relations, the Hamiltonian (1) at a single lattice site can be written as a spin Hamiltonian $H_{\text{spin}} = 2\hbar \Omega J_z$, to within constant energy $\frac{1}{2} \hbar \Omega N (N-1)$. The matrix elements of $H_{\text{spin}}$ for the transitions $|J, m\rangle \rightarrow |J, m+1\rangle$ between the neighbouring magnetic sub-states $(m = -J, \ldots, J)$ are given by $\hbar \Omega \sqrt{(J-m)(J+m+1)}$, which result in a non-dispersive precession of the spin about the field direction with the Larmor frequency $\Omega$ being independent of $J$. Setting formally $J = \frac{1}{2} N$ 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 the states $|N\rangle_a |0\rangle_b$ and $|0\rangle_a |N\rangle_b$ with the same frequency $\Omega$. And in particular, starting from all the atoms in the 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 the state $|b\rangle$.

We now discuss the transfer of a 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

\[
|U_{aa} - \frac{1}{2} (U_{aa} + U_{bb}) \gg \hbar \Omega, \tag{4a}
\]

\[
|U_{aa} - U_{bb} |, |U_{ab} - U_{aa,bb} | \gg \hbar \Omega. \tag{4b}
\]
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 $|n_a⟩$ with $n \neq N$, as clarified below. For convenience, we denote $δU ≡ \left[U_{ab} - \frac{1}{2}(U_{aa} + U_{bb})\right]/\hbar$.

(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 $|a⟩ → |b⟩$, i.e. we set $ω = ω_{ba}$. The field will then induce resonant Rabi oscillations between the states $|1_a, 0_b⟩$ and $|0_a, 1_b⟩$ with frequency $Ω^{(1)} = Ω$. If we apply the field for time $τ^{(1)} = π/2Ω^{(1)}$, resulting in a $π$-pulse, all the single atoms $|1_a⟩$ will be transferred to $|1_b⟩$.

(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 $2ω = 2ω_{ba} + (U_{bb} - U_{aa})/\hbar$, which implies a two-atom (and two-photon) transition $|2_a, 0_b⟩ → |1_a, 1_b⟩ → |0_a, 2_b⟩$ via the nonresonant intermediate state $|1_a, 1_b⟩$ detuned by $δU$. The corresponding two-atom (-photon) Rabi frequency is then $Ω^{(2)} = 2Ω^2/δU$ (the factor of 2 = 2! originates from the double application of the bosonic operators $b^\dagger a$ to the initial state $|2_a, 0_b⟩$), and at time $τ^{(2)} = π/2Ω^{(2)}$, corresponding to an effective $π$-pulse, all the pairs of atoms $|2_a⟩$ will be transferred to $|2_b⟩$.

(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 $3ω = 3ω_{ba} + 3(U_{bb} - U_{aa})/\hbar$, which implies a three-atom (-photon) transition $|3_a, 0_b⟩ → |2_a, 1_b⟩ → |1_a, 2_b⟩ → |0_a, 3_b⟩$ via the nonresonant intermediate states $|2_a, 1_b⟩$ and $|1_a, 2_b⟩$ both detuned by the equal amount $3δU$. The
corresponding three-atom (photon) Rabi frequency is then $\Omega^{(3)} = 6\Omega^2/(2SU)^2$ (the factor of 6 = 3! originates from the triple application of $\hat{b}^\dagger\hat{a}$ to the state $|3,0\rangle$). Note that since both intermediate states $|2,0\rangle$ and $|1,2\rangle$ have the same detuning $2SU$, the second-order ac Stark shifts of the states $|3,0\rangle$ and $|0,3\rangle$ are the same, given by $3\Omega^2/(2SU)$, and the differential shift on the three-photon transition $|3,0\rangle \rightarrow |0,3\rangle$ vanishes. Hence, applying the field for time $\tau^{(3)} = \pi/2\Omega^{(3)}$, corresponding to an effective $\pi$-pulse, all the triplres of atoms $|3,0\rangle$ will be transferred to $|3,0\rangle$.

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 $N\omega = Na_{ba} + \frac{1}{4}N(N-1)(U_{bb} - U_{aa})/\hbar$, the effective $N$-atom (photon) Rabi frequency is then given by

$$\Omega^{(N)} = \frac{N!\Omega^N}{[N(N-1)]^{3/2}U^{-N-1}} = \frac{N\Omega}{(N-1)!} \left( \frac{\Omega}{\delta U} \right)^{N-1}.$$ 

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 the 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 $P_{na}(\tau^{(N)})$ of the final states $|Na\rangle$ at the corresponding times $\tau^{(N)}$ being close to unity, while the probabilities $P_{na}$ of the initial states $|na\rangle$ with $n \neq N$ changing very little during the transfer. For these simulations, we choose $U_{aa}/\hbar \simeq 2\pi \times 10^4 \mathrm{s}^{-1}$, and upon assuming $a_{aa} \simeq a_{bb} \simeq a_{ab}$, $V_a/V_b = 3$ and $\delta r = 0$, obtain from equations (3) $U_{bb} \simeq 0.44U_{aa}$ and $U_{ab} \simeq 0.63U_{aa}$. We then have $\delta U \simeq 2\pi \times 930 \mathrm{s}^{-1}$ and set $\Omega = 2\pi \times 100 \mathrm{s}^{-1}$. The corresponding one-, two- and three-atom transfer times are given, respectively, by $\tau^{(1)} = 2.38 \times 10^{-3} \mathrm{s}$, $\tau^{(2)} = 1.16 \times 10^{-2} \mathrm{s}$ and $\tau^{(3)} = 0.144 \mathrm{s}$, 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 [13–16] or trimers [17] without resorting to more complicated procedures involving the 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 $P_{na}(0) = (n!)e^{-n}/n!$, corresponding to a frozen SF phase with the 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 $\omega$ 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

$$F(N) = \frac{\sum_{n=0}^{N} P_{na}(\tau^{(N)})}{\sum_{n=0}^{N} P_{na}(0)},$$

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 a preselected number of bosonic atoms per site and place them into another internal atomic state, creating thereby a lattice with a desired site occupation number, which we envision to have a number of interesting applications.

Acknowledgment

This work was supported by the EC Marie Curie Research Training Network EMALI.

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