# Particle-hole entanglement of ultracold atoms in an optical lattice 

H. T. Ng<br>Center for Quantum Information, Institute for Interdisciplinary Information Sciences, Tsinghua University, Beijing 100084, P. R. China

(Dated: September 2, 2013)


#### Abstract

We study the ground state of two-component bosonic atoms in a one-dimensional optical lattice. By applying an external field to the atoms at one end of lattice, the atoms are transported and becomes localized at that site. The holes are then created in the remaining sites. The particle-hole superpositions are produced in this process. We investigate the entanglement entropy between the atoms in the two different parts of a lattice. A large degree of particle-hole entanglement is generated in the ground state. The particle-hole quantum correlations can be probed by the two-site parity correlation functions. The transport properties of the low-lying excited states are also discussed.


PACS numbers: 03.75.Gg, 03.75.Lm, $67.85 . \mathrm{Hj}$

## I. INTRODUCTION

Ultracold atoms in optical lattices provide a ground for studying quantum many-body systems 1]. A wide range of interaction parameters of ultracold atomic systems can be tuned 2] and remarkable detection techniques have been demonstrated [3]. For example, a quantum phase transition [2] from a superfluid to a Mott insulator has been shown in ultracold bosons in an optical lattice. Also, high-resolution single-site imaging has been used for probing the Bose-Hubbard model [4].

Recently, particle-hole correlations have been directly observed [5] in a bosonic Mott insulator. Indeed, correlated particle-hole pairs are virtual excitations of a Mott insulator with weak tunnel couplings. Apart from this, the propagation speed of particle-hole correlations of ultracold atoms [6] has been experimentally studied in a one-dimensional (1D) lattice. Such speed of correlations is a fundamental property of the dynamics of a manybody system [7].

In this paper, we consider the ultracold bosonic atoms to be trapped in a 1D lattice as shown in Fig. 11 where a laser field is individually applied to atoms at one end of lattice. Here we consider on-site interactions to be much stronger than the tunnel couplings. The atoms are transported to the site where the field is applied. In fact, the quantum transport of a double-well BoseEinstein condensates by using an external field has been recently discussed [8].

The transport and localization of atoms will create holes in the remaining sites if the system is at unity filling. This situation is different to particle-hole states of the Mott insulator being observed in experiments by Endres et. al [5]. In their experiments, particle-hole excitations can be understood from the first-order perturbation theory [9]. In our case, "real" holes can be created in the lattice by using a local external field. The holes are created in the exact ground state. When a single atom is transported, a superposition of a number of particle-hole states are generated. Therefore, strong particle-hole correlations can build up. These particle-hole correlations can be detected by measuring the two-site parity corre-
lation functions [5, 6].
In addition, we study the entanglement [10] between atoms in the two different parts of a lattice. The entanglement entropy is used to quantify the degree of entanglement. The method of detecting the entanglement entropy in an optical lattice has recently proposed [11, 12]. This quantity can provide useful information of the nontrivial properties of the ground state of a many-body system [13]. We find that a large degree of particle-hole entanglement can be generated when an atom is transported. The ground state becomes highly entangled due to creation of holes. This means that local interactions between the atoms and an external field can give rise to novel behaviours of the ground state.

This paper is organized as follows: In Sec. II, we introduce the model of two-component bosons in an optical lattice and the interactions between atoms and a laser field. In Sec. III, we study the transport of atoms by applying an external field to the atoms. We also investigate the two-site parity correlation functions for detecting the particle-hole correlations. In Sec. IV, we study the entanglement entropy between two parts of the lattice. We discuss the adiabatic transition and the transport properties of the low-lying excited states in Sec. V. Finally, we provide a conclusion.


FIG. 1. (Color online) Atoms in a 1D optical lattice with a harmonic confinement. The local field is individually applied to one end of the lattice with the coupling strength $\Omega$.

## II. SYSTEM

We consider two-component bosonic atoms to be trapped in a 1 D lattice in the presence of a harmonic trap as shown in Fig. [1. Each atom has the two internal states, i.e., the upper state $|e\rangle$ and lower state $|g\rangle$, respectively. This system can be described by the BoseHubbard model [14]. The Hamiltonian of a system of two-component bosons is written as $(\hbar=1)$

$$
\begin{align*}
H= & -\sum_{i=1}^{M}\left(J_{e} e_{i}^{\dagger} e_{i+1}+J_{g} g_{i}^{\dagger} g_{i+1}+\text { H.c. }\right)+U_{e g} \sum_{i=1}^{M} n_{i}^{e} n_{i}^{g} \\
& +\frac{U_{e}}{2} \sum_{i=1}^{M} n_{i}^{e}\left(n_{i}^{e}-1\right)+\frac{U_{g}}{2} \sum_{i=1}^{M} n_{i}^{g}\left(n_{i}^{g}-1\right) \\
& +\sum_{i=1}^{M}\left(\epsilon_{i}^{e} n_{i}^{e}+\epsilon_{i}^{g} n_{i}^{g}\right) \tag{1}
\end{align*}
$$

where $e_{i}^{\dagger}\left(g_{i}^{\dagger}\right)$ and $e_{i}\left(g_{i}\right)$ are the creation and annihilation operators of an atom in the state $|e\rangle(|g\rangle)$ at site $i$, and $M$ is the total number of sites. The parameters $J_{e}\left(J_{g}\right)$ and $U_{e}\left(U_{g}\right)$ are the strengths of tunnel couplings and the atom-atom interactions of atoms in the states $|e\rangle(|g\rangle)$, respectively, and $U_{e g}$ is the strength of inter-component interactions between the atoms. $\epsilon_{i}^{e}$ and $\epsilon_{i}^{g}$ are the strengths of harmonic confinement of the excited and ground states of the atoms, respectively. They are proportional to the square of the distance of the trap centre from their positions [15].

We have assumed that the atoms are trapped in the lowest band of the lattice. In fact, the single-band model is valid [16] provided that the on-site interaction strengths and the temperature are much lower than the energy gap between the first excited band and the lowest band. Apart from this, we consider the interaction strengths between the two component bosons to be approximately equal, i.e., $U_{e e} \approx U_{g g} \approx U_{e g} \approx U$ and $J_{e} \approx J_{g} \approx J$. In fact, the scattering lengths of the two hyperfine spin states of ${ }^{87} \mathrm{Rb}$ are very similar [17].

We consider the atoms to be individually coupled to an external laser field of the frequency $\omega$. In the interaction picture, the Hamiltonian, describes the interaction between the atoms and the laser field, is written as [8]

$$
\begin{equation*}
H_{\mathrm{I}}=\Delta \sum_{i=1}^{M} n_{i}^{e}+\sum_{i=1}^{M} \Omega_{i}\left(e_{i}^{\dagger} g_{i}+\text { H.c. }\right) \tag{2}
\end{equation*}
$$

where $\Delta=\omega-\omega_{g}$ and $\Omega_{i}$ are the detuning and coupling strength between the laser and atom at site $i$, respectively. $\omega_{g}$ is the frequency of the atom in the state $|e\rangle$ and the energy of the ground state $|g\rangle$ is set to be zero. Without loss of generality, we consider the external field to be individually applied to the atoms at the one end of lattice, namely, site $M$.

## III. TRANSPORT AND LOCALIZATION

We study the ground state of the coupled system of the atoms and external field in the strongly interaction regime, i.e., $U \gg J$. We consider that the average number of atoms in each site is equal to one. We employ the exact diagonalization method [18] for numerical simulation. In Fig. 2 2 we plot the number of atoms at site $M$ versus the coupling strength $\Omega$ without the harmonic confinement. The atoms can be transferred to that site $M$ by increasing the coupling strength of the field and atoms. The atoms are transported stepwise 8] around the specific coupling strengths $\Omega_{n}^{*}$ which are given by

$$
\begin{equation*}
\Omega_{n}^{*}=\frac{1}{2}\left[(2 U n+\Delta)^{2}-\Delta^{2}\right]^{1 / 2} \tag{3}
\end{equation*}
$$

The derivation of $\Omega_{n}^{*}$ is given in Appendix A. In the strongly interaction regime, a single atom is only allowed to transport [8]. All atoms can be transferred to site $M$ and becomes localized if $\Omega$ is sufficiently large.

We also study the transport of atoms in the presence of weakly harmonic confinement. In the same figure, we plot the number of atoms at site $M$ as a function of coupling strength $\Omega$ for the different strengths of harmonic confinement. Similarly, the atoms can be transported to site $M$. This shows that the atoms can be transported by applying an external field even if the weakly harmonic confinement is present.


FIG. 2. (Color online) Number of atoms at site $5,\left\langle n_{5}\right\rangle$ versus coupling strength $\Omega$, for $N=M=5, U=20 J$ and $\Delta=0$. The field is applied to the atoms at site 5 . The harmonic confinement strengths $\epsilon_{i}^{e}=\epsilon_{i}^{g}$ are both equal to $(i-3)^{2} \epsilon$. The different parameters $\epsilon$ are denoted by the different lines: $\epsilon=0$ (black-solid), $\epsilon=J$ (blue-dashed) and $\epsilon=2 J$ (reddotted), respectively. The coupling strengths $\Omega_{n}^{*}$ are marked with red arrows.

## A. Particle-hole correlation

Since the system is prepared at unity filling, the localization of atoms leads to creation of holes in the remaining lattice sites. A superposition of particle-hole states


FIG. 3. (Color online) Four different outcomes of particlehole states, where the number of sites $M$ and atoms $N$ are both equal to 5 . The two atoms are localized at the end of the lattice by applying an external field to the atoms at one end of lattice. This causes a hole in the lattice. There are four possible outcomes when a hole is created.
is produced and therefore particle-hole correlations can be generated. The possible outcomes of the system are schematically depicted in Fig. 3. We study the particlehole states between site $M$ and site $M-d$ by calculating the two-site parity correlation function [1, 6] as:

$$
\begin{equation*}
C(d)=\left|\left\langle s_{M} s_{M-d}\right\rangle-\left\langle s_{M}\right\rangle\left\langle s_{M-d}\right\rangle\right|, \tag{4}
\end{equation*}
$$

where $s_{M}=e^{i \pi n_{M}}$ is the parity operator at site $M$ and $d$ is the index of the number of sites between two sites. The quantity $\left\langle s_{i}\right\rangle$ depends on the number of atoms at site $i$. Creation of holes leads to the changes of the number of atoms in each site. Therefore, $C(d)$ can indicate the particle-hole correlations between the two sites.

In Fig. 4 the two-site parity correlations $C(d)$ are plotted as a function of coupling strength $\Omega$. The sharp peaks are shown when $\Omega$ are about $\Omega_{n}^{*}$. This implies that strong particle-hole correlations will be produced when a single atom is transported. Also, the correlation function $C(d)$ decreases when the distance $d$ increases.

## IV. ENTANGLEMENT ENTROPY

We consider a 1D lattice to be bisected into two parts, i.e., the left $L$ and the right $R$ parts, respectively. The subsystem $L$ consists of the number of $M-l$ sites from $1, \ldots, M-l$ and the subsystem $R$ consists of the number of $l$ sites from $M-l+1, \ldots, M$. We study the entanglement between the atoms in the two parts of a lattice.

By using the Schmidt decomposition [10], the ground state $\left|\Psi_{\mathrm{G}}\right\rangle$ can be written as

$$
\begin{equation*}
\left|\Psi_{\mathrm{G}}\right\rangle=\sum_{i} \lambda_{i}\left|\psi^{i}\right\rangle_{L}\left|\psi^{i}\right\rangle_{R} \tag{5}
\end{equation*}
$$

where $\lambda_{i}$ is the Schimdt coefficient. The von-Neumann


FIG. 4. (Color online) Two-site parity correlation, $C(d)$ versus coupling strength $\Omega$, for $N=M=5, U=20 J$ and $\Delta=\epsilon=0$. The different distances $d$ between site $M$ and site $j$ are denoted by the different lines: $d=1$ (black-solid), $d=2$ (blue-dashed) and $d=3$ (red-dotted), and $d=4$ (green-dashdotted) respectively. The coupling strengths $\Omega_{n}^{*}$ are marked with red vertical dashed lines.
entropy [10] is defined as

$$
\begin{equation*}
E(\rho)=-\sum_{i} \lambda_{i}^{2} \ln \lambda_{i}^{2} \tag{6}
\end{equation*}
$$

In Fig. [5] we plot the entanglement entropy $E(\rho)$ versus $\Omega$, for the different sizes $l$. For $l=1$, the entanglement entropy between the particles at site $M$ and holes in the remaining sites is studied. This shows that sharp peaks occur around the coupling strengths $\Omega_{n}^{*}$. This means that a large degree of entanglement is produced when a single atom is transported.

In fact, a large degree of entanglement can also be produced, for $l \geq 1$, as shown in Fig. 5. For example, $E(\rho)$ rises around $\Omega_{n}^{*}$ and becomes flat between $\Omega_{n}^{*}$ and $\Omega_{n+1}^{*}$, for $l=3$. In the limit of large $\Omega$, all atoms becomes localized at site $M$. Then, the entanglement entropy significantly decreases and atoms in the different sites become unentangled in this limit.

## V. DISCUSSION

We study the quantum transport of atoms by adiabatically changing the coupling strength $\Omega(t)=v t$ with the time $t$, where $v$ is a positive number. In Fig. 6, we plot the number of atoms at site $M=3$ versus time, where the number of sites and atoms are both equal to 3 . The atoms are transported stepwise. It is similar to the case of ground state. If the changing rate $v$ is slow enough, then all atoms can be transferred to site 3 . When $v$ becomes larger, the transport rate is faster. But a smaller number of atoms can be transported at site $M$ as shown in Fig. 6

To implement the adiabatic transition, it is necessary to ensure that the changing rate of the parameter $\Omega$ is sufficiently slow [19]. It is required that the changing


FIG. 5. (Color online) Entanglement entropy, $E(\rho)$ versus coupling strength $\Omega$. The same parameters in the previous figure. The subsystem $R$, which consists of the number $l$ of sites, is denoted by the different lines: $l=1$ (black-solid), $l=$ 2 (blue-dashed) and $l=3$ (red-dotted), and $l=4$ (green-dashdotted) respectively. The coupling strengths $\Omega_{n}^{*}$ are marked with red vertical dashed lines.


FIG. 6. (Color online) Number of atoms at site $3,\left\langle n_{3}\right\rangle$ versus time $J t$, for $N=M=3, U=20 J$ and $\Delta=\epsilon=0$. The field is applied to the atoms at site 3 and the coupling strength is a linear function of time, i.e., $v t$. The different values of $v$, are denoted by the different lines: $v=J$ (black-solid), $v=2 J$ (blue-dashed) and $v=3 J$ (red-dotted) respectively.
rate $v$ is much smaller than the energy gap $\Delta E$ between the first excited state and ground state. In Fig. 7 we plot the logarithm of energy gap as a function of $\Omega$. This shows that the energy gap exponentially decreases when the total number $N$ of atoms increases. Therefore, it becomes very difficult to perform the adiabatic transition when $N$ goes large.

To proceed, we study the transport of atoms for the low-lying excited states. In Fig. 8, we plot the number of atoms at site $M$ versus $\Omega$, for the first few eigenstates. The atoms can be transported stepwise when $\Omega$ increases. This method can thus be used for transporting a few atoms when the lattice size grows large. Thus, holes can be created in the remaining lattice sites for the low-lying excited states. The quantum entanglement between the atoms and holes should be generated in a manner similar


FIG. 7. (Color online) Logarithm of $\Delta E$ versus coupling strength $\Omega$, for the different numbers of atoms $N$, and $N=$ $M$. The different number of $N$ are denoted by the different lines: $N=5$ (black-solid), $N=4$ (blue-dashed), $N=3$ (red-dotted) and $N=2$ (gree-dash-dotted), respectively. The parameters are: $U=20 J$ and $\Delta=\epsilon=0$.
to that in the ground state. However, the atoms cannot all be transported to site $M$ for the higher excited states.


FIG. 8. (Color online) Number of atoms at site 5, $\left\langle n_{5}\right\rangle$ versus coupling strength $\Omega$, for the first to fifth eigenstates. The parameters are: $N=M=5, U=20 J$ and $\Delta=\epsilon=0$.

## VI. CONCLUSION

In summary, we have studied the ground state of twocomponent bosons in a 1D optical lattice, where an external field is individually applied to the atoms at one end of the lattice. The atoms can be transported and become localized at that site. In this way, the holes will be created in the remaining sites. The particle-hole correlations can be produced and they can be indicated by two-site parity correlation functions. We have also investigated the entanglement entropy between the atoms in the two parts of a lattice. The large degree of particlehole entanglement can be produced in the ground state. We have discussed the adiabatic transport of the ground state and the transport properties of the low-lying ex-
cited states.

## Appendix A: Transport condition

In this Appendix, we derive the transport condition of atoms for the coupling strengths $\Omega_{n}^{*}$. To obtain the coupling strength $\Omega_{n}^{*}$, it is necessary to find out the groundstate energy of the system. For simplicity, we consider the atoms to be trapped in the lattice without the harmonic confinement, i.e., $\epsilon_{i}^{e}=\epsilon_{i}^{g}=0$.

In the strongly interaction regime, the number of atoms is conserved in each site. We write $S_{i x}=\left(e_{i} g_{i}^{\dagger}+\right.$ $\left.g_{i} e_{i}^{\dagger}\right) / 2, S_{i y}=\left(e_{i} g_{i}^{\dagger}-g_{i} e_{i}^{\dagger}\right) / 2 i$ and $S_{i z}=\left(e_{i}^{\dagger} e_{i}-g_{i}^{\dagger} g_{i}\right) / 2$. The Hamiltonian can be written as

$$
\begin{equation*}
H=\Delta \sum_{i}\left(S_{i z}+\frac{n_{i}}{2}\right)+2 \Omega_{M} S_{M x}+\frac{U}{2} \sum_{i} n_{i}\left(n_{i}-1\right) \tag{A1}
\end{equation*}
$$

where $n_{i}$ is the number operator at site $i$. This Hamiltonian can be diagonalized by applying the transformation to site $M$ :

$$
\begin{align*}
S_{M x} & =\cos \theta S_{M x}^{\prime}-\sin \theta S_{M z}^{\prime}  \tag{A2}\\
S_{M z} & =\cos \theta S_{M z}^{\prime}+\sin \theta S_{M x}^{\prime} \tag{A3}
\end{align*}
$$

and choosing $\Delta \sin \theta+2 \Omega_{m} \cos \theta=0$. The transformed Hamiltonian can be written as

$$
\begin{align*}
H^{\prime}= & \Delta \sum_{i, i \neq M}\left(S_{i z}+\frac{n_{i}}{2}\right)+\frac{\Delta}{2} n_{M}+\sqrt{\Delta^{2}+4 \Omega_{M}^{2}} S_{M z}^{\prime} \\
& +\frac{U}{2} \sum_{i} n_{i}\left(n_{i}-1\right) \tag{A4}
\end{align*}
$$

We consider the number of sites to be larger than or equal to the total number of atoms, i.e., $M \geq N$, then the number of atoms in site $i$ is less than one, where $i \neq M$. In this case, the ground-state energy $E_{G}^{n}$ is

$$
\begin{equation*}
E_{G}^{n}=\frac{\Delta n}{2}-\frac{n}{2} \sqrt{\Delta^{2}+4 \Omega_{M}^{2}}+\frac{U}{2} n(n-1) \tag{A5}
\end{equation*}
$$

where $n$ is the number of atoms in site $M$. The coupling strength $\Omega_{n}^{*}$ can be obtained by considering $E_{G}^{n}=E_{G}^{n+1}$ as

$$
\begin{equation*}
\Omega_{n}^{*}=\frac{1}{2}\left[(2 U n+\Delta)^{2}-\Delta^{2}\right]^{1 / 2} \tag{A6}
\end{equation*}
$$

## ACKNOWLEDGMENTS

H.T.N. thanks Jingning Zhang for useful comment. This work was supported in part by the National Basic Research Program of China Grant 2011CBA00300, 2011CBA00302, the National Natural Science Foundation of China Grant 61033001, 61061130540.
[1] C. Weitenberg, M. Endres, J. F. Sherson, M. Cheneau, P. Schauß, T. Fukuhara, I. Bloch and S. Kuhr, Nature 471, 319 (2011).
[2] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch and I. Bloch, Nature, 415, 39 (2002).
[3] W. S. Bakr, J. I. Gillen, A. Peng, S. Fölling and M. Greiner, Nature, 462, 74 (2009).
[4] W. S. Bakr, A. Peng, M. E. Tai, R. Ma, J. Simon, J. I. Gillen, S. Fölling, L. Pollet, M. Greiner, Science, 329, 547 (2010).
[5] M. Endres, M. Cheneau, T. Fukuhara, C. Weitenberg, P. Schauß, C. Gross, L. Mazza, M. C. Bañuls, L. Pollet, I. Bloch, and S. Kuhr, Science, 334, 200 (2011).
[6] M. Cheneau, P. Barmettler, D. Poletti, M. Endres, P. Schauß, T. Fukuhara, C. Gross, I. Bloch, C. Kollath, and S. Kuhr, Nature, 481, 484 (2012).
[7] E. H. Lieb and D. W. Robinson, Commun. Math. Phys., 28, 251 (1972).
[8] H. T. Ng and S.-I Chu, Phys. Rev. A, 85, 023636 (2012).
[9] E. Toth, A. M. Rey, P. B. Blakie, Phys. Rev. A, 78, 013627 (2008).
[10] R. Horodecki, P. Horodecki, M. Horodecki, K. Horodecki,

Rev. Mod. Phys., 81, 865 (2009).
[11] D. A. Abanin and E. Demler, Phys. Rev. Lett., 109, 020504 (2012).
[12] A. J. Daley, H. Pichler, J. Schachenmayer, P. Zoller, Phys. Rev. Lett., 109, 020505 (2012) .
[13] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett., 90, 227902 (2003).
[14] M. P. A. Fisher, P. B. Weichman, G. Grinstein and D. S. Fisher, Phys. Rev. B, 40, 546 (1989).
[15] M. Greiner, PhD thesis, Ludwig-Maximilian University Munich (2003).
[16] H. Pichler, J. Schachenmayer, A. J. Daley and P. Zoller, Phys. Rev. A, 87, 033606 (2013).
[17] M. R. Matthews, D. S. Hall, D. S. Jin, J. R. Ensher, C. E. Wieman, E. A. Cornell, F. Dalfovo, C. Minniti, and S. Stringari, Phys. Rev. Lett., 81, 243 (1998).
[18] J. M. Zhang and R. X. Dong, Eur. J. Phys., 31, 591 (2010).
[19] A. Messiah, Quantum Mechanics (Dover, New York, 1999).

