Coherent shift of localized bound pairs in the Bose-Hubbard model

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Based on the exact results obtained by Bethe ansatz, we demonstrate the existence of stable bound-pair (BP) wave packet in Bose-Hubbard model with arbitrary on-site interaction U. In large-U regime, it is found that an incoming single-particle can coherently pass through a BP wave packet and leave a coherent shift in the position of it. This suggests a simple scheme for constructing a BP charge qubit to realize a quantum switch, which is capable of controlling the coherent transport of one and *only one* photon in a one-dimensional waveguide.

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I. INTRODUCTION

Most recently, many theoretical and experimental investigations about bound pair (BP) in strongly correlated boson systems are carried out [1–9] since the experimental observation of atomic BP in optical lattice [1]. Counter intuitively, it is found that the trapped rubidium atoms in a three-dimensional optical lattice can form a stable BP, even though in free space the two atoms would have repelled each other. For the problems BP, we can cast back for much earlier investigations of η-pairing states in Hubbard model for electrons, which possess off-diagonal long-range order (ODLRO) [10]. Actually, the basic physics of both fermion and boson BPs is that the periodic potential suppresses the single-particle (SP) tunneling across the barrier, a process that would lead to a decay of the pair. Interesting questions are whether such a BP as composite particle will occur in moderate U system and whether it can exist stably as a wave packet. It is crucial for quantum information processing since the Bose-Hubbard model is the simplest model capturing the main physics of not only cold atoms in optical lattice but also photons in nonlinear waveguide [11–13].

In this paper we will present some exact results obtained by Bethe ansatz concerning the two-particle problem. We demonstrate the existence of a stable BP wave packet in Bose-Hubbard model with arbitrary on-site interaction U. It is found that the most stable BP wave packets refer to different regions of a bound-pair band (BPB) and have different group velocities as U varies from zero to infinity, but spread to the same fidelity when they travel over the same distance. This feature allows the BP wave packet as a new object to be a flying and stationary qubit in quantum device. We also investigate the scattering between a BP wave packet and a single particle in large-U limit. It is found that an incoming SP wave packet can coherently pass through a BP and leave a coherent shift in the position of the BP, which arises from the exotic effective exchange interaction between them. Furthermore, utilizing on-site U one can confine a BP, rather than a SP, in two sites to form a charge qubit. This suggests a simple scheme to realize a quantum switch, which is capable of controlling the coherent transport of one and *only one* photon in a one-dimensional waveguide.

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II. WAVE PACKET IN BOUND-PAIR BAND

The simplest model capturing some physics of the nonlinearity of photons in a coupled-cavity array and cold atoms in optical lattice is a Bose-Hubbard model. The Hamiltonian H is written as follows:

$$H = -\kappa\sum_{i=1}^{N}(a_i^{\dagger}a_{i+1} + \text{H.c.}) + \frac{U}{2}\sum_{i=1}^{N} n_i(n_i - 1), \tag{1}$$

where $a_i^{\dagger}$ is the creation operator of the boson at ith site, the tunneling strength and on-site interaction between bosons are denoted by κ and U. For the sake of clarity and simplicity, we only consider odd-site system with $N=2N_0+1$, and periodic boundary conditions $a_{N+1}=a_1$.

Consider the two-particle problem, a state in the two-particle Hilbert space can be written as

$$|\psi_k\rangle = \sum_{k,r} f^k(r)|\phi_r^k\rangle, \tag{2a}$$

$$|\phi_0^k\rangle = \frac{1}{\sqrt{2N}}e^{i(k/2)}\sum_j e^{ikj}(a_j^{\dagger})^2|\text{vac}\rangle, \tag{2b}$$

$$|\phi_r^k\rangle = \frac{1}{\sqrt{N}}e^{i[k(r+1)/2]}\sum_j e^{ikj}a_j^{\dagger}a_{j+r}^{\dagger}|\text{vac}\rangle, \tag{2c}$$

where $k=2\pi n/N$, $n\in[1,N]$ denotes the momentum, and $r\in[1,N_0-1]$ is the distance between two particles. Due to the translational symmetry of the present system, the Schrödinger equations for $f^k(r)$, $r\in[0,N_0-1]$ is easily shown to be

$$\left[\sum_{j=0}^{N_0-1} T_j^k(\delta_{j,r+1} + \delta_{j,r-1}) - U\delta_{r,0} + T_r^k\delta_{r,N_0} - \varepsilon_k\right]f^k(r) = 0, \tag{3}$$

where $T_r^k=-2\sqrt{2}\kappa\cos(k/2)$ for $r=0$, and $-2\kappa\cos(k/2)$ for $r\neq 0$, respectively. Obviously, for an arbitrary k, the solution of Eq. (3) is equivalent to that of a noninteracting N_0-site tight-binding chain with nearest-neighbor hopping amplitude T_j^k, on-site potentials U, and $-2\kappa\cos(k/2)$ at two ends, respectively. In this work, we focus our study on the bound states. In each k-invariant subspace, there exists only one bound state for nonzero U, which can be obtained via Bethe ansatz method. And all the N bound states, indexed by k, constitute a bound-pair band.

For a large N system, the pair-bound band can be expressed as

$$\varepsilon_k = \mathrm{sgn}(U)\sqrt{U^2 + 16\kappa^2\cos^2\frac{k}{2}} \tag{4}$$

with the wave function

$$f^k(r) \simeq [\mathrm{sgn}(\zeta_k)]^r(1+\zeta_k^2)^{-1/4} \times \begin{cases} 1, & (r=0) \\ \sqrt{2}e^{-|\mu_k|r}, & (r\neq 0) \end{cases}, \tag{5}$$

where $\zeta_k = 4\kappa\cos(k/2)/U$ and $\mu_k = \ln[1/\zeta_k + \sqrt{1+(1/\zeta_k)^2}]$. The spectrum of BP [Eq. (4)] is in agreement with that obtained from the Green's function method [1]. The size of the BP for every bound state can be characterized by

$$\lambda_k = \sqrt{\sum_r |rf^k(r)|^2} = \left|\frac{2\sqrt{2}\kappa}{U}\cos\left(\frac{k}{2}\right)\right|, \tag{6}$$

which depends not only on κ/U but also on k. It can be seen that even for weak U, the size of BP still remains small for long-wave eigenstates, which is crucial for the following discussion. On the other hand, for each eigenstate, the BP is delocalized as a composite particle. Nevertheless, it has been argued that approximately nonspreading wave packet can be achieved by a superposition of eigenstates within a linear region, so as to the populated energy levels are equally spaced [14,15]. Note that there exists a linear region in the vicinity of k_0 in the BPB spectrum [Eq. (4)] for any value of U. Here k_0 is determined by the condition,

$$(\partial^2\varepsilon_k/\partial k^2)_{k=k_0} = 0, \tag{7}$$

or its more explicit form $\cos k_0 = \sqrt{(\eta^2-1)} - \eta$, where $\eta = (U^2/8\kappa^2+1)$. Within such a region, a Gaussian wave packet can be constructed in the form

$$|\Phi(k_0,N_c)\rangle = \frac{1}{\sqrt{\Omega}}\sum_k e^{-(1/2\alpha^2)(k-k_0)^2 - iN_c(k-k_0)}|\psi_k\rangle, \tag{8}$$

where $N_c \in [1,N]$ is the center of it in real space, and $\Omega = \sum_k e^{-(1/2\alpha^2)(k-k_0)^2}$ is the normalization factor. The dynamics of such a wave packet is governed by the effective Hamiltonian,

$$H_{\mathrm{eff}} = \sum_k \tilde{\varepsilon}_k |\psi_k\rangle\langle\psi_k| \tag{9}$$

approximately. Here the effective linear dispersion relation is

$$\tilde{\varepsilon}_k = \varepsilon_{k_0} + v_g(k-k_0), \tag{10}$$

where

$$v_g = \left(\frac{\partial\varepsilon_k}{\partial k}\right)_{k=k_0} = 2\kappa\sqrt{1 - \frac{U^2}{8\kappa^2}\left(\sqrt{1+\frac{16\kappa^2}{U^2}} - 1\right)} \tag{11}$$

is the group velocity of the wave packet [Eq. (8)] in real space.

Now we first investigate the dynamics of such wave packet for any value of U under the linear approximation. Taking the state [Eq. (8)] as an initial state $|\tilde{\Psi}(t=0)\rangle$, its time evolution driven by H_{eff} presents $|\tilde{\Psi}(t)\rangle = e^{-iH_{\mathrm{eff}}t}|\Phi(k_0,N_c)\rangle = e^{i\varphi}|\Phi(k_0,N_c+v_g t)\rangle$. The overall phase factor $e^{i\varphi}$ has no effect on the final result. It is obvious that the wave packet moves along the ring with velocity v_g. In this sense, the time evolution of some states governed by H_{eff} can be described as a spatial translation by the operator $\mathcal{U}(t) = \exp(-ikv_g t) \equiv \mathcal{T}(l)$ with a displacement $l = v_g t$. This shows that the shape of the wave packet in the real space does not change approximately during its travel. However, for the exact time evolution, state $|\Psi(t)\rangle = e^{-iHt}|\Phi(k_0,N_c)\rangle$ is slightly different from state $|\tilde{\Psi}(t)\rangle$ due to the nonlinearity of the dispersion [Eq. (4)]. The overlap between two states that evolve from the same initial wave function under two different Hamiltonians H and H_{eff}, respectively, is defined as the Loschmidt echo (LE) or quantum fidelity $F(t) = \langle\Psi(t)|\tilde{\Psi}(t)\rangle$ which can be employed to depict the deformation of a traveling-wave packet. A straightforward calculation shows that

$$F(t) = \frac{1}{\Omega}\sum_k e^{-(k-k_0)^2/\alpha^2}\cos\left[\frac{1}{6}(k-k_0)^3 v_g t\right], \tag{12}$$

which is based on the fact $(\partial^3\varepsilon_k/\partial k^3)_{k=k_0} = -v_g$.

Remarkably, the fact that the fidelity [Eq. (12)] only depends on $v_g t$ means that the wave packets with fixed α but different k_0 share the same fidelities after they travel the same distance $l = v_g t$. It indicates that a slower wave packet in strong U system has longer life time comparing to a faster one in a weak U system. This feature can be utilized to quantum information processing: weak U system can be a quantum channel for quantum state transfer, while strong U system can be employed for quantum state storage.

The above discussion tells us that a state of type [Eq. (8)] is nonspreading only within certain approximate limits. Next we investigate the profile of such a state in real space. It is well known that for a SP case, if we replace $|\psi_k\rangle$ as $|k\rangle = (1/\sqrt{N})\sum_j e^{ikj}a_j^\dagger|\mathrm{vac}\rangle$, the SP wave function is

$$|\phi(k_0,N_c)\rangle = \frac{1}{\sqrt{\Omega}}\sum_j e^{-(\alpha^2/2)(j-N_c)^2 + ik_0 j}a_j^\dagger|\mathrm{vac}\rangle, \tag{13}$$

which is also a wave packet of Gaussian type [15]. For two-particle state [Eq. (8)], its profile in real space can be described by the distribution of the average particle density,

$$\langle n_i(t)\rangle = \langle\Psi(t)|a_i^\dagger a_i|\Psi(t)\rangle = |a_i|\Psi(t)\rangle|^2. \tag{14}$$

In Fig. 1(a) we plot $\langle n_i(t)\rangle$ for the wave packets with $\alpha = 2/15$ at time $t=0$ and $\tau = 15/\kappa$ in the systems with $U=0.1$, 0.5, 1, 5, 10, and 20 in the unit of κ. It shows that the profile of the wave packets in the real space is also Gaussian type and nonspreading. It also indicates that the shape of the wave

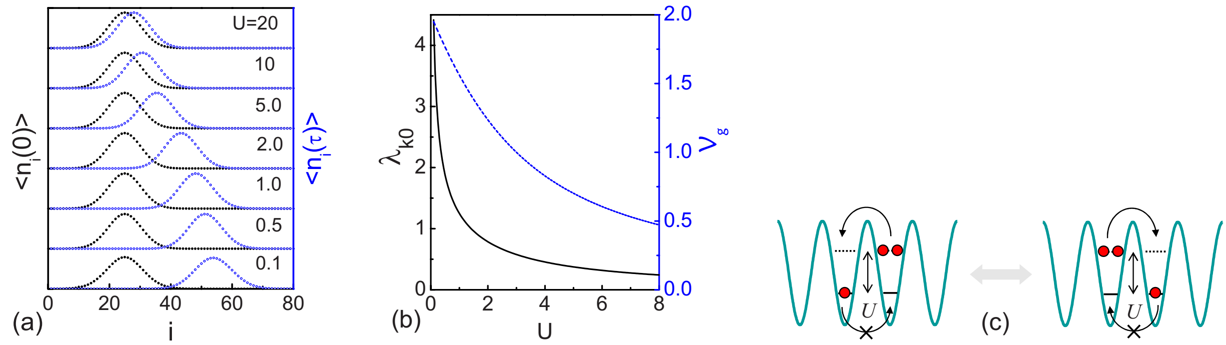

FIG. 1. (Color online) (a) Plots of $\langle n_i(t)\rangle$ the wave packets with $\alpha=2/15$ at time $t=0$ (dot) and $t=\tau=15/\kappa$ (empty circle) in the systems with $U=0.1-20$ in the unit of κ. (b) Plots of v_g in the unit of κ (dashed line) and size λ_{k_0} (solid line) for the BP Gaussian wave packets. (c) Schematic of the exchange interaction between SP and BP.

packets does not change apparently for different U, which is in agreement with the following observation from Eq. (15) that the size of a BP remains small for $|U|\gtrsim 0.2\kappa$.

For a given α, the size of a composite particle in the form of a nonspreading wave packet is a function only of the ratio κ/U,

$$\lambda_{k_0}=\frac{1}{\sqrt{2}}\sqrt{\sqrt{1+\frac{16\kappa^2}{U^2}}-1},\qquad(15)$$

which determines the size of the wave packet. To demonstrate the features of a BP wave packet for arbitrary U system, its velocity v_g and size λ_{k_0} are plotted in Fig. 1(b). For $U/\kappa=0.2-10$, we have $\lambda_{k_0}=0.2-3.1$, which is sufficiently small that we can have many pairs in the lattice without having substantial overlap between them. It implies a new phase, a gas of BPs which has been predicted in large U limits [3], can also exist in moderate U system. It is worthy to stress that, although a SP wave packet [Eq. (13)] and a BP wave packet [Eq. (8)] share some common properties, on-site interaction U is able to govern a BP rather than a SP wave packet. In this sense, the SP and BP wave packets can be regarded as two different types of particles. Nevertheless the interaction between them is exotic since the constituent of BP is essentially SP.

III. COHERENT SHIFT

In the following we restrict ourselves to large U limit. Consider a three-body problem. The spectrum consists of three bands around 0, U, and $3U$. We are interested in the middle band, which corresponds to a SP and a BP. Using perturbation method, the corresponding effective Hamiltonian is

$$\widetilde{H}=-\kappa\sum_{i=1}^{N}\widetilde{a}_i^\dagger\widetilde{a}_{i+1}+\frac{2\kappa^2}{U}\sum_{i=1}^{N}\widetilde{b}_i^\dagger\widetilde{b}_{i+1}-2\kappa\sum_{i=1}^{N}\widetilde{b}_{i+1}^\dagger\widetilde{b}_i\widetilde{a}_i^\dagger\widetilde{a}_{i+1}+\text{H.c.}+U\sum_{i=1}^{N}\widetilde{b}_i^\dagger\widetilde{b}_i,\qquad(16)$$

where $\widetilde{a}_i$ and $\widetilde{b}_i$ denote the hardcore bosons satisfying the following commutation relations:

$$[\widetilde{a}_j,\widetilde{a}_i^\dagger]=[\widetilde{b}_j,\widetilde{a}_i^\dagger]=[\widetilde{b}_j,\widetilde{b}_i^\dagger]=0\quad(i\neq j),$$

$$\{\widetilde{a}_i,\widetilde{a}_i^\dagger\}=\{\widetilde{b}_i,\widetilde{b}_i^\dagger\}=1;\{\widetilde{b}_i,\widetilde{a}_i^\dagger\}=\{\widetilde{b}_i,\widetilde{a}_i\}=0.\qquad(17)$$

The first two terms describe the hopping of SP and BP, the third term describes the interaction between the two kinds of particles, the process of which is schematically illustrated in Fig. 1(c). Now we focus on the scattering between SP and BP wave packets. In short-time duration, a BP is relative stationary comparing with a moving SP wave packet. Then the swapping operation $\widetilde{b}_{i+1}^\dagger\widetilde{b}_i\widetilde{a}_i^\dagger\widetilde{a}_{i+1}$ allows the incoming SP wave packet to "pass through" the BP and shift its position with a unit lattice spacing. To demonstrate this process, numerical simulation is performed for the time evolution of such two wave packets. The initial state is $|\phi(\pi/2,N_{\text{SP}})\rangle|\Phi(\pi/2,N_{\text{BP}})\rangle$ with $N_{\text{SP}}\ll N_{\text{BP}}$. In the simplest case of replacing the swapping term 2κ by κ, the final state is $|\phi(\pi/2,N_{\text{SP}})\rangle|\Phi(\pi/2,N_{\text{BP}}-1)\rangle$ with $N_{\text{SP}}\gg N_{\text{BP}}$. Actually, factor 2 can cause a slight reflection of the incoming SP wave packet from the above fact. Figure 2 is the stroboscopic picture of the profiles of two evolving wave packets obtained

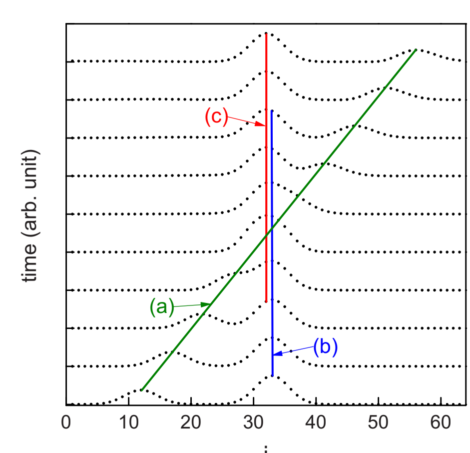

FIG. 2. (Color online) The stroboscopic picture of the profiles of evolving SP and BP wave packets obtained by numerical simulations: line (a) denotes the center of SP wave packet, while lines (b) and (c) denote the centers of BP wave packets before and after scattering.

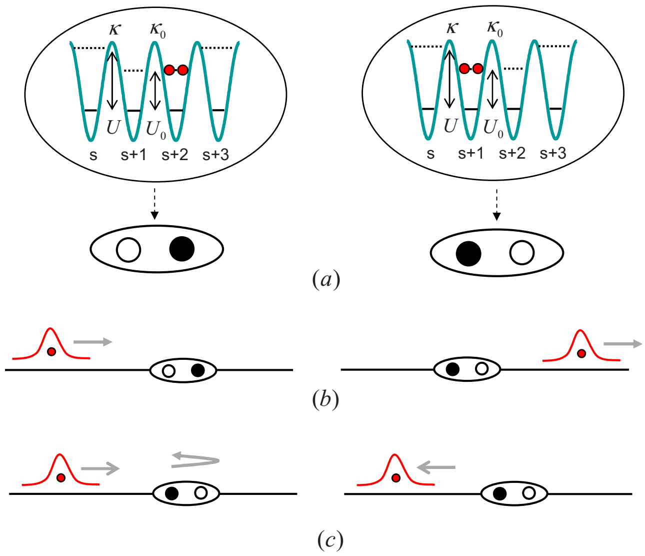

FIG. 3. (Color online) (a) A confined BP as a charge qubit with states $|R\rangle$ and $|L\rangle$. [(b) and (c)] A BP qubit as a quantum switch to control the transport of a SP wave packet. In the case with the qubit in state $|R\rangle$, a moving SP wave packet will pass through the qubit freely but leaves the qubit to be in the $|L\rangle$ state. In contrast, if the qubit is in state $|L\rangle$, the coming wave packet will be totally reflected and remains the qubit to be in state $|L\rangle$.

by numerical simulations for the Hamiltonian (16): line (a) denotes the center of SP wave packet, while lines (b) and (c) denote the centers of BP wave packets before and after scattering. It is clear that the incoming SP wave packet keeps the same speed during the whole process, while the BP wave packet get a coherent shift with a unit of lattice spacing.

Bound-pair charge qubit

Now we apply the novel feature of coherent shift of a BP to construct a quantum switch. Considering a four-site chain in strong on-site interaction limit, the dynamics of a SP and a BP obeys the Hamiltonian

$$H_{CQ} = -\kappa(\widetilde{a}_s^{\dagger}\widetilde{a}_{s+1} + \widetilde{a}_{s+2}^{\dagger}\widetilde{a}_{s+3}) - \kappa_0\widetilde{a}_{s+1}^{\dagger}\widetilde{a}_{s+2} + \frac{2\kappa_0^2}{U_0}\widetilde{b}_{s+1}^{\dagger}\widetilde{b}_{s+2} - 2\kappa_0\widetilde{b}_{s+1}^{\dagger}\widetilde{b}_{s+2}\widetilde{a}_{s+2}^{\dagger}\widetilde{a}_{s+1} + \text{H.c.} + U\sum_{i=s,s+3}\widetilde{b}_i^{\dagger}\widetilde{b}_i + U_0\sum_{i=s+1,s+2}\widetilde{b}_i^{\dagger}\widetilde{b}_i, \tag{18}$$

which is schematically illustrated in Fig. 3(a). We focus on the case of that there is a single BP in the site $s+1$ and $s+2$, which can be realized under the condition $U \gg U_0$. Notice that this setup is equivalent to the system of confining a composite in an effective double-well potential and can be regarded as a charge qubit. Such a qubit has a novel feature due to the coherent shift induced by the scattering with a SP. To demonstrate this, we take $2\kappa_0 = \kappa$ for simplicity and study the dynamical process via time evolution. We embed such a charge qubit into a chain as illustrated in Figs. 3(b) and 3(c). Let us first assume that initially the qubit is in the "right" state $|R\rangle = \widetilde{b}_{s+2}^{\dagger}|\text{vac}\rangle$, while a SP wave packet of type [Eq. (13)] $|\phi(\pi/2, N_c < s)\rangle \equiv |\phi(\pi/2, L)\rangle$ [similarly, we define $|\phi(\pm\pi 2, N_c > s+2)\rangle \equiv |\phi(\pm\pi/2, R)\rangle$] is coming from the left. Comparing to the speed of the SP wave packet $v_g = 2\kappa$, state $|R\rangle$ can be regarded as a stationary state during the whole scattering process. Then according to the Hamiltonian H_{CQ}, the incoming wave will pass through the qubit freely but leaves the qubit to be in the "left" state $|L\rangle = \widetilde{b}_{s+1}^{\dagger}|\text{vac}\rangle$, i.e.,

$$|\phi(\pi/2, L)\rangle|R\rangle \rightarrow |\phi(\pi/2, L)\rangle|L\rangle. \tag{19}$$

In contrast, if the qubit is in state $|L\rangle$, the scattering process is

$$|\phi(\pi/2, L)\rangle|L\rangle \rightarrow |\phi(-\pi/2, L)\rangle|L\rangle, \tag{20}$$

i.e., the incoming wave packet is totally reflected and the qubit remains to be in state $|L\rangle$. These two processes are illustrated schematically in Figs. 3(b) and 3(c). Remarkably, if a sequent wave packets scatter with the BP qubit in $|R\rangle$ state, the first one can pass freely, but the subsequent ones will be reflected totally. This suggests a simple scheme to realize a quantum switch to control the coherent transport of a photon in a one-dimensional waveguide. The photon blockade [16] can be utilized to construct a photon-pair qubit in coupled-cavity array. Nevertheless, different from schemes in Refs. [17,18], our scheme allows one and only one photon passing over the switch.

IV. CONCLUSION

In conclusion, we have studied the existence of localized BP in Bose-Hubbard model with arbitrary on-site interaction U. We have shown that BP wave packets refer to different regimes of a bound-pair band and have different group velocities as U varies from zero to infinity, but spread to the same fidelity when they travel over the same distance. It proposed a new object to be a flying or stationary qubit in quantum device. Furthermore, the coherent shift in large-U system suggests a BP qubit as a quantum switch embedded in a one-dimensional waveguide. Our analysis can be extended to a fermion Hubbard system with a minor correction.

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[1] K. Winkler, G. Thalhammer, F. Lang, R. Grimm, J. Hecker Denschlag, A. J. Daley, A. Kantian, H. P. Büchler, and P. Zoller, Nature (London) **441**, 853 (2006).
[2] S. M. Mahajan and A. Thyagaraja, J. Phys. A **39**, L667 (2006).
[3] D. Petrosyan, B. Schmidt, J. R. Anglin, and M. Fleischhauer, Phys. Rev. A **76**, 033606 (2007).
[4] C. E. Creffield, Phys. Rev. A **75**, 031607(R) (2007).
[5] A. Kuklov and H. Moritz, Phys. Rev. A **75**, 013616 (2007).
[6] S. Fölling, S. Trotzky, P. Cheinet, M. Feld, R. Saers, A. Widera, T. Müller, and I. Bloch, Nature (London) **448**, 1029 (2007).
[7] S. Zöllner, H. D. Meyer, and P. Schmelcher, Phys. Rev. Lett. **100**, 040401 (2008).
[8] L. Wang, Y. Hao, and S. Chen, Eur. Phys. J. D **48**, 229 (2008).
[9] M. Valiente and D. Petrosyan, Europhys. Lett. **83**, 30007 (2008); J. Phys. B **41**, 161002 (2008).
[10] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989).
[11] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
[12] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature (London) **415**, 39 (2002).
[13] M. J. Hartmann, F. G. S. L. Brandão, and M. B. Plenio, Nature Phys. **2**, 849 (2006); M. J. Hartmann and M. B. Plenio, Phys. Rev. Lett. **99**, 103601 (2007).
[14] Y. Li, Z. Song, and C. P. Sun, Commun. Theor. Phys. **48**, 445 (2007).
[15] S. Yang, Z. Song, and C. P. Sun, Phys. Rev. A **73**, 022317 (2006).
[16] K. M. Birnbaum, A. Boca, R. Miller, A. D. Boozer, T. E. Northup, and H. J. Kimble, Nature (London) **436**, 87 (2005).
[17] D. E. Chang, A. S. Sørensen, E. A. Demler, and M. D. Lukin, Nat. Phys. **3**, 807 (2007).
[18] L. Zhou, Z. R. Gong, Y. X. Liu, C. P. Sun, and F. Nori, Phys. Rev. Lett. **101**, 100501 (2008).