Experimentally accessible reentrant phase transitions in double-well optical lattices

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We study the quantum phases of bosons confined in a combined potential of a one-dimensional double-well optical lattice and a parabolic trap. We apply the time-evolving block decimation method to the corresponding two-legged Bose-Hubbard model. In the absence of a parabolic trap, the system of bosons in the double-well optical lattice exhibits a reentrant quantum phase transition between Mott insulator and superfluid phases at unit filling as the tilt of the double-wells is increased. We show that the reentrant phase transition occurs also in the presence of a parabolic trap and suggest that it can be detected in experiments by measuring the matter-wave interference pattern.

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FIG. 1: (color online) Schematic double-well lattice potential in the \(xz\) plane for \(\alpha = 0.2, \theta = 0\), showing the existence of isolated two-legged ladders.

Recently, the system of ultracold bosonic atoms in a double-well optical lattice (DWOL) has been used to study quantum information processing and quantum many-body systems \(^1\),2,3,4. A DWOL is constructed from two-color two-dimensional (2D) lattices in the horizontal \(xy\) plane and another lattice in the vertical \(z\) direction, resulting in a 3D lattice whose unit cell is a double well. By exploiting precise control of the properties of the double wells, recent experiments have realized an atom interferometer \(^2\), two-atom exchange oscillations, which were used to create a quantum SWAP gate \(^3\), and correlated tunneling of two interacting atoms \(^4\).

In single-well optical lattices, the transition from a superfluid (SF) phase to a Mott insulator (MI) phase has been observed by adiabatically increasing the lattice depth \(^2\,5\). In previous DWOL experiments all the double wells were independent of each other due to the large potential barrier between them, and the system was always in an insulating phase. However, the potential barrier could be lowered to induce a transition to a SF phase \(^1\). In particular, one can investigate the SF-MI transition in a two-legged ladder 1D DWOL by tuning the lattice depth in the vertical direction. While in single-well lattices the SF-MI transition is determined by the ratio, \(U/t\), of the on-site interaction energy to the hopping energy \(^5\,6\), in DWOL the SF-MI transition is governed by the competition between the on-site interaction and the tilt (energy offset) of the double wells.

In this paper, we study the ground state properties of bosons in a two-legged ladder lattice with a parabolic confining potential. This case is more representative of current experiments than is an unconfined, homogeneous lattice. Although mean-field-type methods describe the SF-MI transition of bosons in optical lattices very well in 3D \(^2\), they fail to describe quantitatively the two-legged ladder system due to strong quantum fluctuations \(^5\). Hence, we use the time-evolving block decimation (TEBD) method \(^9\,10\), which is one of the best methods currently available to study strongly correlated 1D quantum systems. We show here that a reentrant phase transition (MI-SF-MI) occurs as the tilt of the double wells is changed for a fixed parabolic confinement. Moreover, a distinctive signature of the reentrant phase transition appears in the momentum distribution, which is directly related to matter-wave interference patterns observed in experiments.

We consider a Bose gas at zero temperature confined in a combined potential of a DWOL and a parabolic trap. A DWOL potential in Refs. \(^1\,2\,3\) is given by

\[
V(r) = V_{\text{in}} \left( \sin^2(kx) + \sin^2(ky) - 2 \right) - V_{\text{out}} \left( \sin(kx - \theta) + \cos(ky) \right)^2 + V_s \sin^2(kz),
\]

where \(V_{\text{in}}\) is the depth of the “in-plane” lattice with period of \(d \equiv \pi/k\), whose light polarization is in the \(xy\) plane, \(V_{\text{out}}\) the depth of the “out-of-plane” lattice with 2\(d\)-periodicity \(^1\), and \(V_s\) is the depth of the lattice in the vertical \(z\) direction. When the ratio \(\alpha \equiv V_{\text{out}}/V_{\text{in}}\) satisfies \(0 < \alpha < 0.5\), the unit cell of the potential Eq. \(^1\) is a double-well. Control of the ratio \(\alpha\) and the relative phase \(\theta\) provides the flexibility to adjust the double-well parameters: the barrier height and the tilt. When \(\theta = 0\), the double wells are symmetric (no tilt). Increasing \(\alpha\) from zero enlarges the barrier height \(V_{\text{high}}\) between double wells in the \(xy\) plane and reduces the barrier height \(V_{\text{low}}\) between two wells within a double well. Keeping
$V_{\text{high}} - V_{\text{low}} \gg E_R$ and tuning $V_z$, one can create an ensemble of 1D DWOLs with a two-legged ladder structure, where all the two-legged ladders are decoupled from each other as shown in Fig. 1. Here $E_R = \frac{\hbar^2 k^2}{2m}$ is the recoil energy, where $m$ is the boson mass.

At zero temperature the many-body quantum state of interacting bosons in an optical lattice is well described by the Bose-Hubbard model when the lattice is so deep that only the lowest energy level of each lattice site is occupied and tunneling occurs only between nearest-neighboring sites [11, 12]. To study bosons in 1D DWOLs, we use the two-legged Bose-Hubbard Hamiltonian (BHH)

$$ H = \sum_j \left\{ \sum_{\eta \in \{L,R\}} \left( \frac{U}{2} \hat{n}_{j,\eta}(\hat{n}_{j,\eta} - 1) + (\Omega j^2 - \mu)\hat{n}_{j,\eta} ight) - t_{\parallel}(\hat{a}_{j+1,\eta}^{\dagger}\hat{a}_{j,\eta} + \text{h.c.}) - t_{\perp}(\hat{a}_{j,R}^{\dagger}\hat{a}_{j,L} + \text{h.c.}) + \frac{\lambda}{2}(\hat{n}_{j,L} - \hat{n}_{j,R}) \right\}. $$

(2)

$a_{j,\eta}^{\dagger}$ creates a boson at the lowest level localized on the left (right) of the $j$-th double-well for $\eta = L(R)$, and $\hat{n}_{j,\eta} = a_{j,\eta}^{\dagger}a_{j,\eta}$ is the number operator. The lattice parameters can be related to the DWOL depths $V_{\text{in}}, V_{\text{out}},$ and $V_z$ and the recoil energy $E_R$ by assuming that $\theta \ll 1$ and that each well is sufficiently deep to approximate the Wannier function by a Gaussian. In this case, the on-site interaction is $U \sim E_R (8\pi)^{1/2} a_{\eta} (1 - 2\alpha)/\sqrt{\Omega} s_{z,\eta}/4$; the intrachain hopping is $t_{\parallel} \sim E_R \left( \frac{1}{2} - 1 \right) s_\eta e^{-\pi^2 s_\eta/4}$; and the interchain hopping is $t_{\perp} \sim E_R \left( \frac{1}{\sqrt{2}} - 2 \cot \left( \frac{\alpha}{2} \right) - 1 + 2a_\eta \right) e^{-f(\alpha)\sqrt{\pi}/\theta}$. Here, $\alpha = V_{\text{out}}/V_{\text{in}}$, $s = V_{\text{in}}/E_R$, $a_\eta = V_z/E_R$, $a_\eta$ is the s-wave scattering length, and $f(\alpha) = \frac{\alpha}{\cos \left( \frac{\alpha}{2} \right)}$. $\Omega$ is the curvature of the parabolic trap, and $\mu$ is the chemical potential, which controls the total number of bosons $N$. Notice that $U$, $t_{\parallel}$, and $t_{\perp}$ are approximately independent of the tilt as long as $\theta \ll 1$.

We now describe briefly the zero-temperature phase diagrams of the two-legged Bose-Hubbard model with no confining potential ($\Omega = 0$) [8, 13, 14]. In Figs. 2a)-(c), we show the phase diagrams in the $(\mu/U, t_{\parallel}/U)$ plane for $t_{\perp}/U = 0.1$. We see the usual MI phase with unit filling, $\nu = 1$ (corresponding to two atoms per double well), and also one with half filling, $\nu = 1/2$, [8, 13]. The SF-MI phase boundary in the $(\mu/U, t_{\parallel}/U)$ plane significantly depends on $t_{\parallel}/U$ [14] and $\lambda/U$ [8]. In particular, the unit-filling MI phase depends nonmonotonically upon $\lambda/U$. As seen in the upper lobes of the phase diagrams, the $\nu = 1$ MI region shrinks initially as $\lambda/U$ is increased from zero. The size of the MI region is minimized at $\lambda = U$, where the local states $|1,1\rangle$ and $|0,2\rangle$ are nearly degenerate; $|n_L,n_R\rangle$ designates the local Fock state with $n_L(n_R)$ bosons on the left (right) of a double well. Due to this degeneracy, coherence is developed within each double well and the system favors the SF phase. As $\lambda/U$ is increased further, the MI region grows again. This nonmonotonic behavior leads to a reentrant phase transition from a MI to a SF and again to a MI, induced by increasing $\lambda/U$.

Since we are mainly interested in the reentrant phase transition, we investigate how the ground state properties change with increasing $\lambda/U$ for the following fixed values of the other parameters: $N = 98$, $\Omega/U = 0.001$, $t_{\parallel}/U = 0.1$, and $t_{\perp}/U = 0.05$. This value of $t_{\parallel}/U$ is sufficiently small such that the MI domain with $\nu = 1$ is present when $\lambda = 0$ or $\lambda \gg U$, while it is so large that the $\nu = 1$ MI domain is absent when $\lambda = U$. The number of double wells is chosen as $L = 85$. This value of $L$ is so large that the bosons do not see the edge of the system.

To analyze the two-legged BHH [2], we use the finite-size version of the TEBD method [3], which provides a precise ground state for 1D quantum lattice systems via propagation in imaginary time. While the maximum
number of bosons per site is $N_{\text{max}} = \infty$, convergence is already achieved in our numerical calculations when $N_{\text{max}} = 5$. We calculate the ground states of the Hamiltonian (2) with $\chi = 80$, where $\chi$ is the size of the basis set retained in the TEBD procedure [9].

In Fig. 3 we show the density profile $\bar{n}_j = n_{j,L} + n_{j,R} = \sum_\eta \langle \hat{n}_{j,\eta} \rangle$, namely the local number of bosons in the $j$-th double well as a function of $\lambda/U$. For $\lambda = 0$, the system is essentially a plateau with unit filling ($\bar{n}_j = 2$), with small SF regions with incommensurate filling at the edges. This plateau indicates the presence of an incompressible MI domain [5, 13, 15, 16, 18]. As $\lambda/U$ is increased, the unit-filling plateau starts to melt at a certain point and a new MI plateau with half filling ($\bar{n}_j = 1$) emerges. In the vicinity of $\lambda = U$, the unit-filling plateau has been completely melted away and the density profile for $\bar{n}_j > 1$ is smooth, with the reflected parabolic shape of the confining potential that is characteristic of SF phases in the regime where the local density approximation is valid [13]. As $\lambda/U$ is increased further, the unit-filling plateau forms again at the center of the system. Thus, as in the homogeneous case, the reentrant phase transition is caused by increasing the tilt parameter in the presence of a parabolic potential [14].

For a better understanding of the reentrant phase transition, three slices from Fig. 3 are shown in Figs. 2(d)-(f) as functions of $\lambda/U$. This means the intrachain coherence increases as the SF phase transition occurs, which is small in the MI regions and almost vanishes, namely $n_{j,L} \simeq 0$ for $\bar{n}_j < 1$. In contrast, a considerable amount of bosons remains in the left well as $n_{j,L} \simeq \bar{n}_j^{-1}/2$ for $\bar{n}_j > 1$, since the local state with unit-filling is approximately given by $|1,1 \rangle + |0,2 \rangle / \sqrt{2}$ due to the competition between the onsite interaction and the tilt. At $\lambda = 2U$, the population of bosons in the left well almost vanishes, namely $n_{j,L} \simeq 0$, in the entire system.

Next, we calculate the quasi-momentum distribution $S(k) = L^{-1} \sum_{j,l} \sum_\eta e^{ik\hat{d}j} \langle \hat{n}_{j,\eta}^{\dagger} \hat{a}_{l,\eta} \rangle$, where $\hat{d}$ is the lattice spacing. Since the true-momentum distribution is expressed as the product of $|w(k)|^2$ and $S(k)$ [18], where $w(k)$ is the Fourier transform of the Wannier function in the lowest Bloch band, the quasi-momentum distribution can be extracted by dividing the true-momentum distribution observed in experiments by $|w(k)|^2$ [4]. $S(k)$ is shown as a function of $\lambda/U$ in Fig. 4(a), where the $k = 0$ peak is the sharpest in the vicinity of $\lambda = U$. This means the intrachain coherence increases as the SF region around the trap center emerges.

To quantify the sharpness of the peak in $S(k)$, we cal-
We calculate first the local coherence $\langle a_j^\dagger a_{j,R} \rangle$ as shown in Fig. 5(a). At $\lambda = 0$, since the local state with half-filling is well approximated by the bonding state, the SF regions at the boundary of the trapped gas have large local coherence. As $\lambda/U$ is increased, the region with $\bar{n}_j \leq 1$ immediately loses the local coherence. In contrast, in the region with $\bar{n}_j > 1$ the local coherence is pronouncedly large at $\lambda = U$. The development of local coherence is due to the degeneracy of $|1,1\rangle$ and $|0,2\rangle$ states, and it drives the system into the SF phase. As $\lambda/U$ is increased further, the entire system tends to lose coherence. In Fig. 5(b), the total coherence $C$ is shown as a function of $\lambda/U$. While the total coherence is significantly reduced when $\lambda$ is increased from $U$, it hardly changes in the region $\lambda < U$. This happens because the gain of local coherence for $\bar{n}_j > 1$ and the loss for $\bar{n}_j \leq 1$ almost cancel each other out. Consequently, the double-slit diffraction pattern can not capture the signature of the reentrant phase transition.

In conclusion, we have studied the SF-MI transition of parabolically trapped Bose gases in a 1D double-well optical lattice by using the time-evolving block decimation (TEBD) method. We have calculated the density profile as a function of the tilt of the double wells and shown that a reentrant phase transition between MI and SF phases occurs in the presence of a parabolic confinement. We have calculated also the quasi-momentum distribution and found that the matter-wave interference pattern, which is one of the most common observables in experiments with cold atoms, contains sufficient information to characterize the reentrant phase transition. We would like to emphasize that, unlike the results of mean-field theories, our results based on the TEBD method are quantitative, thus we expect the reentrant phase transition to be observed in future experiments near the parameter values discussed in this paper.

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