Self trapping in the two-dimensional Bose-Hubbard model

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We study the expansion of harmonically trapped bosons in a two-dimensional lattice after suddenly turning off the confining potential. We show that, in the presence of multiple occupancies per lattice site and strong interactions, the system exhibits a clear dynamical separation into slowly and rapidly expanding clouds. We discuss how this effect can be understood within a simple picture by invoking doublons and Bose enhancement. This picture is corroborated by an analysis of the momentum distribution function in the regions with slowly and rapidly expanding bosons.

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In contrast to standard time-of-flight measurements after turning off all trapping and optical lattice potentials, in which the role of interactions can either be accounted for in a straightforward way or neglected, recent theoretical [11–13, 15] and experimental [19, 20] studies have shown that expanding interacting particles in low-dimensional geometries and/or in the presence of lattice potentials can lead to surprising and interesting effects [see Ref. [21] for a review of some of these effects in one dimension (1D)]. Among those, and of particular relevance to this work, have been the observation of emerging (quasi)coherent correlations during the expansion of Mott insulators in 1D [11, 13, 15] and higher-dimensional [12, 13] lattices, as well as self-trapping and quantum distillation of fermions [9] and bosons [11] in 1D.

Expansions of fermions [19] and bosons [20] have also been studied in optical lattices in experiments. In the fermionic case, the systems were prepared in a band-insulating state and expansion dynamics were studied for different values (and signs) of the on-site interaction. Remarkably, it was found that the dynamics transitions from ballistic at very weak interactions to bimodal (a slowly expanding spherical core was surrounded by a ballistically expanding square-shaped cloud) with increasing interactions. Qualitatively similar results were obtained for bosons initially prepared in a Fock state (with interactions. Qualitatively similar results were obtained for different values (and signs) of the on-site interaction. Motivated by those results, we study the expansion of bosons with repulsive interactions in the presence of multiple occupancies. We show that, within a mean-field approximation, the system dynamically separates into slowly and rapidly expanding clouds, similar to what has been seen in experiments. Our results emphasize the importance of self-trapping [11] in the presence of multiple occupancies and strong interactions in two dimensions (2D).

We consider 2D lattice bosons modeled by the Bose-Hubbard model [22] with an additional harmonic trap

\[ \hat{H} = -J \sum_{\langle i,j \rangle} \left( \hat{a}_i^\dagger \hat{a}_j + \text{H.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \sum_i (V_i - \mu) \hat{n}_i, \]  

where standard notation has been used [3]. \( V_i = V r_i^2 \) models the harmonic potential (with strength \( V \)), and \( r_i \) (to be given in units of the lattice spacing) is the distance of site \( i \) with respect to the center of the trap.

We study the expansion dynamics after turning off the confining potential (\( V = 0 \)) at time \( t = 0 \). By selecting \( U/J \) to be smaller than the mean-field critical value \( (U/J)_c \approx 23.31 \) for the formation of the \( n = 1 \) Mott insulator (we select \( U/J \leq 23 \)), the initial state is always taken to be in a superfluid phase with an on-site density \( 1 \leq n_{\text{center}} \leq 2 \) at the center of the trap. Note that \( U \) and \( J \) are not changed when the trap is turned off. The expansion dynamics are studied using the time-dependent Gutzwiller mean-field approximation [4, 24].

In Fig. 1, we show results for the density profiles in systems with two different values of the on-site interaction \( U/J = 15 \times 15 \) (panels) and \( U/J = 23 \times 23 \) (panels) for different times after turning off the trap. For the times shown, it can be seen that a significant number of bosons remain in the region where \( n > 1 \) at all times (dubbed “slowly expanding cloud”), while the rest of the cloud expands (dubbed “rapidly expanding cloud”). A comparison between the results for \( U/J = 15 \) and \( U/J = 23 \) makes apparent that this effect is strengthened when the interaction strength is increased. For strong interactions, such a self-trapping can be partially understood to be a consequence of energy conservation, which forbids the breakup of a double occupancy (doublon) because the resulting excess energy cannot be released into the system [27]. Furthermore, pairs of adjacent doublons effectively attract each other, thus increasing the stability of the central \( n > 1 \) region. The latter is the result of an energy gain due to virtual tunneling transitions between individual bosons belonging to two adjacent doublons [18, 28, 29]. Within this picture, a region with dominant doublon occupation can expand only in a time scale \( \propto J^2/U \), due to second order tunneling processes.

On the other hand, bosons that expand into the empty lattice do so in a ballistic manner resembling the one observed during the expansion of a Mott insulator with \( n = 1 \) [3]. There, the fastest expansion was seen along the diagonals, where the fastest group velocity can develop in this geometry. This effect is accentuated as the
interaction strength is increased. As mentioned above, a similar bimodal expansion in which a nonexpanding core was surrounded by ballistically expanding particles (with a square-shaped distribution) has been observed in recent experiments that considered different initial states for fermions and bosons.

Another noticeable characteristic of the slowly expanding cloud (Fig. 1) is that its site occupancies fluctuate in space and time, and even reach values that are greater than those in the initial state. This is similar to the quantum distillation process observed in fermions in one dimension, in which doublons grouped together in the center of the system. However, in contrast to the latter case, full distillation (all doublons forming a cluster) does not occur here. Figure 1 indicates (n is always smaller than two), and an analysis of single occupancies confirms, that a fraction of the bosons that remain in the slowly expanding cloud are in singly occupied sites (monomers).

The fact that bosonic monomers can remain in the slowly expanding cloud while fermionic ones do not is a consequence of Bose enhancement, as argued for the one-dimensional case in Ref. 9. Extending those arguments to two dimensions, this can be understood as follows. In the presence of strong repulsive interactions, the dispersion relation of bosons within the region of density n \leq 1 is, to a good approximation, the same as that of hard-core bosons in the vacuum \( \epsilon_{k,\exp} = -2J(\cos k_x + \cos k_y) \) [3, 11]. In contrast, within the slowly expanding cloud where n > 1, monomers (again approximated by hard-core bosons) propagate via resonant single-particle hopping with a Bose enhanced amplitude J' = 2J. Thus, the dispersion relation of monomers is \( \epsilon_{k,\exp} = -4J(\cos k_x + \cos k_y) \). This means that in the rapidly expanding cloud bosons have \( \epsilon_{k,\exp} \in [-4J, 4J] \) while in the slowly expanding cloud monomers have \( \epsilon_{k,\exp} \in [-8J, 8J] \). Thus, only monomers with energies in the center of the band, \(-4J \leq \epsilon_{k,\exp} \leq 4J\), are able to escape into the rapidly expanding cloud because their energies match those of bosons in the vacuum. This leads to four relations that define the momenta of bosons that can leave the slowly expanding cloud,

\[
k_y \geq \pm \arccos(\pm 1 - \cos k_x),
\]

\[
k_y \leq \pm \arccos(\mp 1 - \cos k_x).
\]  

Obviously, this can only (if at all) approximate what happens in a real system where interactions are finite and many-body effects are expected to affect the dynamics. In what follows, we look for signatures of the scenario above in the dynamics of the momenta occupations.

In Fig. 2, we show the momentum distribution function for the same systems and times depicted in Fig. 1. While they exhibit a rich structure, there are two specific features that are worth highlighting. The first one is that, at all times, there is a high population of modes close to \( k_x = k_y = 0 \), i.e., there is a sizable fraction of bosons that either do not move or do so very slowly. The second one is that, during the expansion and with increasing \( U/J \), a high population develops in modes with \( k_y = \pi \pm k_x \) and \( k_y = -\pi \pm k_x \). The latter ones are the modes that become most highly populated during the expansion of a Mott insulator with \( n = 1 \) in the same geometry considered here. They account for the fastest moving particles along the diagonals. This already suggests that different features in the momentum distribution may be associated to the slowly and rapidly expanding clouds seen in the density profiles in Fig. 1 which we now study.

Figure 2 shows the momentum distribution of bosons that are part of the slowly (left) and rapidly (right) expanding clouds for \( U/J = 23 \). In our calculations, as a slowly expanding cloud we take the bosons that remain in the region where at \( t = 0 \) the system had \( n > 1 \). (We find this to be a reasonable working definition despite the fact that, as seen in Fig. 1, the region with \( n > 1 \) does shrink during the expansion.) For \( U/J = 23 \), the slowly expanding cloud consists of bosons that remain in a circle of radius \( r_{\text{slow}} = 8.5 \) (in units of the lattice spacing) at the center of the system. The rest of the bosons were taken to be the rapidly expanding cloud. The right panels in Fig. 2 show that the momentum distribution of the rapidly expanding cloud develops a diamondlike structure with a small population of the...
modes around \( k = 0 \). This structure becomes better defined as \( U/J \) increases and is similar to the one observed during the expansion of a Mott insulator \(^3\).

More interestingly, the left panels in Fig. 3 show that, in addition to an almost uniformly populated background, particles in the slowly expanding cloud predominantly occupy low-momentum modes. Those modes belong to the \( k \)-space region for which monomers are not allowed to escape \(^2\). This confirms the relevance of the scenario proposed. During the dynamics, one can also see that the population of the momentum modes changes due to interactions, which allow some monomers to fall in the \( k \) region where they can escape. Interactions are also important in the rapidly expanding cloud, where redistribution of momenta also occurs (right panels in Fig. 3).

Overall, and similarly to results found in Refs. \(^3, 5, 13\), it is remarkable that the scenario previously discussed, which was developed for \( U \rightarrow \infty \), provides a good qualitative understanding of the expansion of Bose-Hubbard systems with finite values of \( U \) (greater than the bandwidth).

We have studied the expansion of systems with values of \( U/J \) between 1 and 23, and initial site occupancies in the center of the trap between 1.0 and 2.0, and have found that the self-trapping phenomenon discussed before occurs in an extended domain of interactions and fillings. Summarizing our results, Fig. 4(a) depicts the ratio \( P \) between the time-averaged number of particles that remain in the slowly expanding cloud at times \( t \approx 30\hbar/J \) (longest time simulated as particles reach the edges of our lattice) and the number of particles that were there initially vs \( U/J \) and \( n_{\text{center}} \) at \( t = 0 \). At those long times \( t \), \( P \) exhibits a very weak time dependence.

Figure 4(a) shows that, for weak interactions (\( U/J < 5 \)), there is essentially no slowly expanding cloud for all initial densities \( n_{\text{center}} \) considered. Under such conditions, doublons are not well-defined entities and self-trapping does not occur. As \( U/J \) increases beyond the bandwidth, self-trapping starts to occur at lower occupancies in the center of the trap. This is expected as doublons become more difficult to break and less of them will dissociate and abandon the central region. Furthermore, the scenario presented for the trapping of monomers becomes more relevant as \( U/J \) increases, which further increases the stability of the region with \( n > 1 \).

In recent experiments \(^19, 20\), a quantity of much interest has been the core expansion velocity and
FIG. 4. (Color online) (a) Percentage of particles \( P \) that remain in the slowly expanding region at times \( t \simeq 30 \hbar /J \), at which the fastest escaping particles have started reaching the edges of the 100 \( \times \) 100 lattice utilized in our calculations [26], and (b) average radial expansion velocity \( \bar{v}_r \) at times \( t \simeq 15 \hbar /J \), at which it is almost time independent [26], versus \( n_{\text{center}} \) and \( U/J \). For all systems, \( V/J = 0.161 \). \( \bar{v}_r \) is given in units of lattice spacing times \( J/\hbar \).

its alternative measure, the radial expansion velocity \( v_r(t) = (d/dt) \sqrt{R^2(t) - R^2(0)} \), where \( R^2(t) = (1/N) \sum_i \langle \hat{n}_i(t) \rangle r_i^2 \) and \( N \) is the total number of particles. We have calculated \( v_r(t) \) for all cases for which results were presented in Fig. 4(a). In general, this quantity is found to exhibit a transient regime in the early stages of the expansion and stabilizes to values that do not depend strongly on time before particles start reaching the edges of the lattice [26]. Figure 4(b) depicts our results for such a stable radial velocity.

In Fig. 4(b) one can see that, in the weakly interacting regime, \( v_r(t) \) is low and slowly increases as the occupancy in the center of the trap increases. However, as \( U/J \) increases, this velocity exhibits a maximum and steadily decreases as \( n_{\text{center}} \) increases further. The initial increase can be intuitively understood as more interaction energy is present in the initial state and that energy is transformed into kinetic energy during the expansion. On the other hand, when \( U/J \) exceeds a certain \( n_{\text{center}} \)-dependent value, the self-trapping mechanism discussed before sets in and the velocity starts to decrease. As expected, the value of \( U/J \) at which the latter happens decreases with increasing filling and correlates with the onset of trapping in Fig. 4(b).

Note that the radial expansion velocities starting from the ground state of the trapped system are found to be nonzero as long as one is not deep in the self-trapping regime. This is in contrast to the experimental results for two-dimensional lattice bosons in Ref. [20] where, after a quench in the interaction strength, it was found that the radial expansion velocities drop quickly to zero as one moves away from the noninteracting limit. An important question that remains to be addressed, either theoretically with unbiased approaches or experimentally in the absence of an interaction quench, is whether starting from the ground state of a trapped two-dimensional system one obtains zero or nonzero radial expansion velocities. Independently of the possible outcome of those studies, the self-trapping effect studied here within the mean-field approximation is expected to be robust, and has already been explored in one dimension [13, 20].

In summary, we have shown that the expansion of bosons in a two-dimensional lattice, after turning off a trap, can lead to a dynamical separation of the gas into a slowly and rapidly expanding clouds. The onset of this phenomenon depends on the ratio \( U/J \) and the number of double occupancies at \( t = 0 \), and was related to the difficulty of breaking doublons in the presence of strong repulsive interactions. We have also shown that, in contrast to the fermionic case, Bose enhancement can lead to the trapping of monomers. Furthermore, we analyzed the effect that self-trapping has on the radial expansion velocity of the system, which could be potentially studied in experiments with ultracold bosons in optical lattices.

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A. Gutzwiller mean-field approximation

The results presented in the main text were obtained using the Gutzwiller mean-field approximation, discussed in detail in Refs. [1–4]. Within this approach, the ground state and time-evolving states are approximated by a product of individual site wavefunctions, each of which is a linear combination of Fock states:

\[ |\psi_{MF}\rangle = \prod_{i=1}^{L} \sum_{n=0}^{n_c} \alpha_{in} |n\rangle_i \]  

(3)

Here, \( L = l \times l \) is the total number of lattice sites and \( l \) is the linear size, \( |n\rangle_i \) is a Fock state corresponding to \( n \) particles at site \( i \), \( n_c \) is the cutoff determining the maximum number of particles allowed per site (\( n_c = 5 \) in our study), and \( \alpha_{in} \) are the coefficients associated with each Fock state. The ground state of the system is obtained by finding the coefficients \( \alpha_{in} \) that minimize the mean-field energy. The equations for the time evolution of the coefficients \( \alpha_{in} \) during the expansion are obtained utilizing the time-dependent variational principle [1–4], and we integrate them numerically using a fourth-order Runge-Kutta with a discretization time \( \delta t = 2.0 \times 10^{-4} \).

B. Momentum distributions for \( U/J = 15 \)

Figure 6 shows the time evolution of the momentum distribution function of the slowly and rapidly expanding clouds in a system with \( U/J = 15 \). The momentum distribution function is computed by Fourier transforming the one-particle density matrix as

\[ n_{k}^{\beta}(t) = \frac{1}{L} \sum_{i,j} e^{i\hat{k}(r_{i} - r_{j})} \langle \psi_{MF}^{\beta}| b_{i}^\dagger b_{j}| \psi_{MF}^{\beta} \rangle, \]

(4)

where the sums go over the entire lattice, \( r_{i} \) is the position of the \( i \)-th site in the lattice, and \( \beta = s, r \) indicates whether we are dealing with the slowly or rapidly expanding cloud, respectively. The mean-field states \( |\psi_{MF}^{\beta}\rangle \), written in terms of new sets \( \alpha_{in}^{\beta} \), are defined through the full set of coefficients \( \alpha_{in} \) in Eq. (3) and the radius of the

Supplementary Materials:
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FIG. 5. (Color online) Momentum distribution function of the slowly (left panels) and rapidly (right panels) expanding clouds for $U/J = 15$, and the same times depicted in Figs. 1 and 2 in the main text. White curves demarcate regions in momentum space for which monomers can or cannot escape the slowly expanding cloud (see main text).

circle defining the slowly expanding cloud $r_{\text{slow}}$. For the slowly expanding region they are defined as

\[
\begin{align*}
\alpha_{in}^s & = \alpha_{in} \quad \text{if } |r_i| \leq r_{\text{slow}}, \\
\alpha_{i0}^s & = 1 \quad \text{if } |r_i| > r_{\text{slow}}, \\
\alpha_{in \neq 0}^s & = 0 \quad \text{if } |r_i| > r_{\text{slow}},
\end{align*}
\]

while for the rapidly expanding region they are defined as

\[
\begin{align*}
\alpha_{in}^r & = \alpha_{in} \quad \text{if } |r_i| \geq r_{\text{slow}}, \\
\alpha_{i0}^r & = 1 \quad \text{if } |r_i| < r_{\text{slow}}, \\
\alpha_{in \neq 0}^r & = 0 \quad \text{if } |r_i| < r_{\text{slow}},
\end{align*}
\]

The results for the time evolution of the density profiles and full momentum distributions of this system were shown in Figs. 1 and 2 in the main text. We note that at $t = 0$, and later times, the occupation of some momentum modes may exceed the scale depicted in Fig. 5 and in the figures in the main text. We have truncated those occupancies at 0.5 so that the most important features in the momentum distribution function can be discerned in the plots.

The results depicted in Fig. 5 are qualitatively similar to those for $U/J = 23$ in Fig. 3 in the main text. The most apparent quantitative difference is that the diamond-like structures in the expanding cloud are significantly more populated for $U/J = 23$ than for $U/J = 15$. This is expected from the analysis in Ref. [3].

C. Radial expansion velocity

Figure 6 shows the time evolution of the radial expansion velocity after turning off the trap for $U/J = 18$ and two different values of $n_{\text{center}}$ [Fig. 6(a)] and for $n_{\text{center}} = 1.8$ and two different values of $U/J$ [Fig. 6(b)]. One can see there that, after a transient regime, the velocities become almost time independent before dropping abruptly when particles start reaching the edges of the lattice.

For fixed $U/J = 18$, Fig. 6(a) shows that an increase in $n_{\text{center}}$ from 1.4 to 1.8 results in a decrease in the radial expansion velocity. This is understandable as the initial number of doublons increases, which enhances self trapping. For fixed $n_{\text{center}} = 1.8$, Fig. 6(b) shows that an increase in $U/J$ from 10 to 18 also causes $v_r(t)$ to decrease. This is because doublons become more difficult to break and self trapping is also enhanced. These two effects were discussed in the main text in the context of the results presented in Fig. 4(b).
D. Percentage of slowly expanding particles and asymptotic radial expansion velocity

Figure 7(a) shows the evolution of the percentage of particles $P$ initially confined that remain in the slowly expanding region at times $t \approx 30\hbar/J$ as a function of $n_{\text{center}}$ and for several values of $U/J$. $P$ is computed as a time average over 15 time steps, from $t = 28.6\hbar/J$ to $t = 30.0\hbar/J$ (every $t = 0.1\hbar/J$). For small values of $U/J < 2$ there are no particles that remain in the slowly expanding region for any initial occupancy at the center of the lattice, whereas for larger values of $U/J$ there is a finite amount of particles that remain in the slowly expanding cloud for large enough $n_{\text{center}}$. The value of $n_{\text{center}}$ at which the self-trapping sets in decreases as the interaction $U/J$ is increased, as expected.

![Percentage of particles remaining (a) and radial expansion velocity (b)](image)

Figure 7(b) shows the time-averaged radial expansion velocity $\bar{v}_r$ at times $t \approx 15\hbar/J$. The average velocity is given in units of lattice spacing times $J/\hbar$.

Figure 7(a) shows the evolution of the percentage of particles $P$ initially confined that remain in the slowly expanding region at times $t \approx 30\hbar/J$ as a function of $n_{\text{center}}$ and for several values of $U/J$. $P$ is computed as a time average over 15 time steps, from $t = 28.6\hbar/J$ to $t = 30.0\hbar/J$ (every $t = 0.1\hbar/J$). For small values of $U/J < 2$ there are no particles that remain in the slowly expanding region for any initial occupancy at the center of the lattice, whereas for larger values of $U/J$ there is a finite amount of particles that remain in the slowly expanding cloud for large enough $n_{\text{center}}$. The value of $n_{\text{center}}$ at which the self-trapping sets in decreases as the interaction $U/J$ is increased, as expected.

E. Radially averaged densities after a long expansion time

Figure 8 depicts the radially averaged density profiles after $t = 20\hbar/J$ for several values of $U/J$ as a function of the distance from the center of the system. Notice that the density profiles in this study do not possess radial symmetry and some information is lost by taking the radial average. Nevertheless, such information can be contrasted directly with experiments and helps to detect the onset of self-trapping.

Figure 8 shows that, for small values of $U/J = 4, 8$, there is no self-trapping in the time scales considered. For $U/J = 12, 16$, on the other hand, self-trapping does occur. The data in this figure are consistent with Fig. 4 of the main text, for which, at $n_c = 1.5$, self-trapping becomes apparent at $U/J \approx 10$.

![Radially averaged density profiles](image)

Figure 8. (Color online) Radially averaged density profiles after $t = 20\hbar/J$ for different values of $U/J$. The distance is given in units of the lattice spacing. The initial site occupancy at the center of the trap was taken to be $n_c = 1.5$ and the strength of the trapping potential to be $V/J = 0.161$.

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