Expansion dynamics in two-dimensional Bose-Hubbard lattices: BEC and thermal cloud

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(Dated: July 13, 2020)

We study the temporal expansion of an ultracold Bose gas in two-dimensional, square optical lattices. The gas is described by the Bose-Hubbard model deep in the superfluid regime, with initially all bosons condensed in the central site of the lattice. We use the previously developed nonequilibrium propagator method for capturing the time evolution of an interacting bosonic system, where the many-body Hamiltonian is represented in an appropriate local basis and the corresponding field operators are separated into the classical (BEC) part and quantum mechanical fluctuations. After a quench, i.e. after a sudden switch of the lattice nearest-neighbor hopping, the expanding, bosonic cloud separates spatially into a fast, ballistic forerunner and a slowly expanding central part controlled by selftrapping. We show that the forerunner expansion is driven by the coherent dynamics of the BEC and that its velocity is consistent with the Lieb-Robinson bound. For smaller lattices we analyze how quasiparticle collisions lead to enhanced condensate depletion and oscillation damping.

I. INTRODUCTION

The Bose-Hubbard model has been in the focus of condensed matter research since the seminal paper by Fisher et al. [1], which predicted a superfluid–Mott-localization transition, and especially after its experimental realization in ultracold atom systems [2]. It is well known that systems of cold atoms encompass a number of impressive advantages over their solid state counterparts, among which are the full system controllability, freedom from impurities, isolation from the environment, and last but not least, the possibility to realize quantum quenches. A quantum quench, i.e. an abrupt change of one of the system’s parameters, is a controlled way to bring a system out of equilibrium and to study its nonequilibrium dynamics and potential thermalization [3].

The temporal expansion of clouds of interacting, bosonic atoms in optical lattices has been studied experimentally in ultracold atom systems in 1D and 2D. In the experiment [11] a Mott insulating core with unity filling was prepared in the center of a two-dimensional (2D) optical lattice. By abruptly lowering the lattice depth in one or both directions, tunneling and correspondingly expansion of the boson gas was induced and studied in detail in dependence on the interaction strength $U$. It was found that both dimensionality and interaction play an important role in the nonequilibrium expansion dynamics. In particular, the expansion in a 2D lattice developed bimodal cloud shapes with slow dynamics in the round, central part of the cloud surrounded by fast, square-shaped ballistic wings. The core expansion velocity slowed down with the growth of interaction and eventually saturated [4]. On the theoretical side, expansion dynamics in more than one spatial dimension has so far been studied on the level of mean-field theories [5,7], that is, considering the dynamics of the Bose-Einstein condensate (BEC) and neglecting the influence of the thermal cloud or incoherent excitations. In particular, time-dependent Gutzwiller mean-field theory was employed to analyze the expansion dynamics in 2D bosonic Mott-Hubbard lattices [5,7,8]. It was found, that initially confined Mott-insulating states become coherent during the expansion after removal of a confining potential [5], and initially superfluid states with small occupation numbers expand in a bimodal way with a central, slowly expanding cloud surrounded by a rapidly expanding low-density cloud of bosons [6]. The Bosons expand ballistically and fastest along the diagonals of the lattice. The physics behind the expansion behaviour was attributed to the fact, that the central cloud consists predominantly of doublons, which tend to group together [9], whereas the fast expanding part consists of monomers [6].

However, previous studies of the quench dynamics of Bose-Josephson junctions (BJJ) [10,11] showed that incoherent fluctuations become inevitably excitated after the quench even in gapped systems, due to the finite spectral distribution involved in the temporal evolution. The coupling of the BEC to these incoherent excitations plays an important role in the relaxation and thermalization dynamics [12,13]. Exact numerical calculations of the expansion dynamics are possible only in one dimension [4,15], where true Bose-Einstein condensation does not occur and, hence, a distinction between BEC and incoherent excitations is not possible in the time-dependent situation.

To tackle the problem of the expansion of the coupled system of BEC and incoherent fluctuations we, therefore, adopt the semi-analytical formalism developed earlier and
applied for studies of nonequilibrium BJJ's \[10\] \[12\] \[13\]. Our approach goes beyond mean-field approximations and systematically takes into account incoherent excitations. It consists of coupled equations of motion for the classical, space-time dependent BEC amplitudes and for the full Keldysh quantum propagators of the noncondensate fluctuations. These equations are derived from a generating functional using the Keldysh-Kadanoff-Baym nonequilibrium approach \[19\] \[10\] \[17\], which leads to a hierarchy of conserving approximations, and are solved self-consistently. We focus on the expansion dynamics of weakly interacting bosons in two dimensions, deep in the superfluid phase. For large square lattices of size $21 \times 21$, we evaluate the theory within the leading-order in $U$ conserving approximation, the Bogoliubov-Hartree-Fock (BHF) approximation, while for smaller system size $(3 \times 3)$ we use the second-order selfconsistent approximation, thus taking inelastic relaxation processes into account. Unlike previous treatments \[5\] \[6\] we can consider arbitrary large numbers of particles within our formalism. Note however that we do not attain the Mott localized phase since the interactions are assumed to be weak.

As the main results we find that even for small interaction strength but large values of the initial local occupation number the coherent part of the expanding cloud splits into two modes, a slowly expanding high-density central part and a fast expanding low-density pulse or “forerunner”. In this case of high-occupation number, however, the expansion of the high-density part is not inhibited by doublon formation \[5\] but by the interaction-induced selftrapping effect known from the oscillation dynamics of BJJ's \[10\] \[18\] \[19\]. The forerunner expands ballistically, typical for coherent waves. These results are in good agreement with experiments on 2D expansion \[4\]. The forerunner's expansion speed is largest along the lattice diagonals where it obeys and reaches the Lieb-Robinson bound \[20\]. The latter states that there is a finite limit to the speed of information propagation in any quantum system.

In addition, we are able to distinguish the dynamics of the incoherent excitation cloud from the coherent one. The density of incoherent excitations increases with the interaction strength $u$, as expected, but with increasing $U$ it ceases to participate in the forerunner. This confirms that the forerunner is a coherence phenomenon. Taking inelastic two-particle scattering into account for small lattices beyond the BHF approximation, we find that it leads to fast damping of density oscillations between the BEC and the incoherent fluctuations and to enhanced depletion of the condensate.

This article is organized as follows. In chapter \[11\] we describe our model and derive the general kinetic equations based on the Keldysh-Kadanoff-Baym nonequilibrium approach. Section \[11\] \[13\] contains the equations of motion without two-particle damping, i.e., the dynamical BHF approximation, while in section \[11\] \[14\] the collision integrals describing inelastic interactions are taken into account. The results within the BHF approximation and including inelastic processes are presented and discussed in detail in sections \[11\] and \[11\] \[14\] respectively. We conclude in section \[15\].

II. MODEL AND EQUATIONS OF MOTION

A. General kinetic equations

We consider ultracold bosons in a 2D, square optical lattice described by the Bose-Hubbard Hamiltonian \[21\]

$$H = -J(t) \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \sum_i (\epsilon_i - \mu) \hat{b}_i^\dagger \hat{b}_i + \frac{U}{2} \sum_i n_i (n_i - 1),$$

where $J(t) = J \Theta(t)$ is the nearest neighbor hopping amplitude which is abruptly switched on at time $t = 0$, $U$ is the repulsive interaction between bosons, and $\mu$ the chemical potential. $\hat{b}_i^\dagger, \hat{b}_i$ are bosonic creation and annihilation operators on site $i$ and $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ the boson number operator. Hereafter we will consider a homogeneous lattice, $\epsilon = \epsilon_i$ for any $i$. As initial conditions at $t = 0$ we assume all bosons condensed deep in the superfluid phase and trapped by a tight confining potential in the central site of the lattice.

After the tunneling $J(t)$ is turned on for $t > 0$, two main processes set in: (i) the superfluid part is allowed to expand in all direction of the lattice; (ii) incoherent excitations get excited and are expanding along with the superfluid part. We analyze the resultant dynamics using the formalism developed earlier \[10\] \[11\] based on standard nonequilibrium techniques \[16\] \[22\] \[23\]. As usual we decompose the bosonic operators into their expectation or saddlepoint value $a_i(t) = \langle \hat{b}_i \rangle$ and the fluctuations $\tilde{\varphi}_i$, $\tilde{\varphi}_i$, $\hat{b}_i = a_i(t) + \tilde{\varphi}_i$, $\hat{b}_i^\dagger = a_i^*(t) + \tilde{\varphi}_i^\dagger$, (2)

where $a_i(t)$ represents the local BEC amplitude and the noncondensate quantum fluctuations are described by the operators $\tilde{\varphi}_i = \hat{b}_i - a_i(t)$ obeying canonical bosonic commutation relations. We now treat the condensate amplitudes semiclassically and the quantum fluctuations quantum field-theoretically in order to capture the nonequilibrium dynamics. The full bosonic propagator splits into two parts $C + G$, with

$$C_{ij}(t,t') = -i \left( a_i(t) a_j^*(t') \langle a_i(t) a_j(t') \rangle \right),$$

$$G_{ij}(t,t') = \left( \begin{array}{cc} T_C \hat{b}_i(t) \hat{b}_j^\dagger(t') \langle T_C \hat{b}_i(t) \hat{b}_j^\dagger(t') \rangle \\ T_C \hat{b}_i^\dagger(t) \hat{b}_j(t') \langle T_C \hat{b}_i^\dagger(t) \hat{b}_j(t') \rangle \end{array} \right)，$$

where $T_C$ denotes time-ordering operator along the Keldysh contour and $i$ the imaginary unit. The general
Dyson equations for the propagators $C$ and $G$ read,

\[
\sum_k \int \frac{d\tau}{C} \left[ G_{0,i,k}(t,\tau) - C^{HF}(t,\tau) \right] C_{kj}(\tau,t') = \sum_k \int \frac{d\tau}{C} S_{ik}(t,\tau) C_{kj}(\tau,t'), \\
\sum_k \int \frac{d\tau}{C} \left[ G_{0,i,k}(t,\tau) - \Sigma_{ik}^{HF}(t,\tau) \right] G_{kj}(\tau,t') = i \delta(t-t')\delta_{ij} + \sum_k \int \frac{d\tau}{\Sigma_{ik}} G_{kj}(\tau,t').
\]

(5)(6)

Here, all integrals as well as the Dirac $\delta(t-t')$ are defined along the Keldysh contour $C$. For convenience, we also separate the selfenergy into two parts: the local Hartree-Fock (HF) part and the collision part, described by $S$ and $\Sigma$, respectively [11][13]. The inverse bare propagator reads

\[
G_{0,i,j}^{-1}(t,t') = \left[ i \tau_3 \delta_{ij} \frac{\partial}{\partial t} + J(\delta_{i,j+1} + \delta_{i,j-1}) \right] \delta(t-t'),
\]

(7)

where $I$ and $\tau_3$ denote the unit and the third Pauli matrix in Bogoliubov particle-hole space, respectively. For the further analysis it is convenient to rewrite the general Dyson equations [3], [4] in terms of symmetrized and antisymmetrized field-correlation functions,

\[
A_{ij}(t,t') = i \left[ G_{ij}^>(t,t') - G_{ij}^<(t,t') \right] = \begin{pmatrix} A^G_{ij} F^F_{ij} \\ A^F_{ij} F^G_{ij} \end{pmatrix},
\]

\[
F_{ij}(t,t') = \frac{1}{2} \left[ G_{ij}^>(t,t') + G_{ij}^<(t,t') \right] = \begin{pmatrix} F^G_{ij} F^F_{ij} \\ F^F_{ij} F^G_{ij} \end{pmatrix},
\]

(8)

where we omitted the time arguments in the matrix representations for simplicity. Similarly, we introduce for the selfenergies,

\[
\gamma_{ij}(t,t') = i \left[ S_{ij}^>(t,t') - S_{ij}^<(t,t') \right] = \begin{pmatrix} \gamma^G_{ij} \gamma^F_{ij} \\ \gamma^F_{ij} \gamma^G_{ij} \end{pmatrix},
\]

\[
\Gamma_{ij}(t,t') = i \left[ \Sigma_{ij}^>(t,t') - \Sigma_{ij}^<(t,t') \right] = \begin{pmatrix} \Gamma^G_{ij} \Gamma^F_{ij} \\ \Gamma^F_{ij} \Gamma^G_{ij} \end{pmatrix},
\]

\[
\Pi_{ij}(t,t') = \frac{1}{2} \left[ \Sigma_{ij}^>(t,t') + \Sigma_{ij}^<(t,t') \right] = \begin{pmatrix} \Pi^G_{ij} \Pi^F_{ij} \\ \Pi^F_{ij} \Pi^G_{ij} \end{pmatrix}.
\]

(9)

The symbols "<" and "->" refer to the standard "lesser" and "greater" notations for nonequilibrium Green’s functions and selfenergies [23].

With these new notations we can rewrite Eqs. [3], [4] in terms of symmetrized and antisymmetrized correlators and their selfenergies

\[
i \tau_3 \frac{\partial}{\partial t} C_{ij} = -J(C_{i+1,j} + C_{i-1,j}) + S_{ij}^{HF} C_{ij} - i \sum_k \int_0^t d\tau \gamma_{ik} C_{kj},
\]

(10)

\[
i \tau_3 \frac{\partial}{\partial t} A_{ij} = -J(A_{i+1,j} + A_{i-1,j}) + \Sigma_{ij}^{HF} A_{ij} - i \sum_k \int_{\tau}^t d\tau \Gamma_{ik} A_{kj},
\]

(11)

\[
i \tau_3 \frac{\partial}{\partial t} F_{ij} = -J(F_{i+1,j} + F_{i-1,j}) + \Sigma_{ij}^{HF} F_{ij} - i \sum_k \int_{\tau}^t d\tau \Pi_{ik} A_{kj}.
\]

(12)

Here, we used the locality of the Hartree-Fock selfenergies in the time arguments as well as in the site indices, i.e. $S_{ij}^{HF} = S_{i}^{HF} \delta_{ij}(t-t')$ and similar for $\Sigma_{ij}^{HF}$, and evaluated the contour integrals. Because of the quench boundary conditions, the integrals involving collisional selfenergies in Eqs. (10)-(12) start from 0 and not from $-\infty$. For simplicity, we omitted again explicit time arguments of the Green’s functions and selfenergies, The argument $t$ refers to the first argument of the functions and selfenergies, that is, $C_{ij} \equiv C_{ij}(t,t')$ and $\int_{\tau}^t d\tau \Pi_{ik} A_{kj} = \int_{\tau}^t d\tau T_{ik} \int_{\tau}^t A_{kj}(t',t')$, etc. The boundary conditions are formulated in such a way that the system of equations (10)-(12) becomes an initial value problem.

B. Bogoliubov-Hartree-Fock approximation

In this section we specify the set of differential equations derived from (10)-(12) in BHF approximation, i.e. the first-order in $U$ conserving approximation [22]. To first order in $U$ we neglect the integrals in Eqs. (10)-(12) and explicitly calculate the HF selfenergies $S_{ij}^{HF}$ and $\Sigma_{ij}^{HF}$ as

\[
\Sigma_{i}^{HF} = \left( \Sigma_{i}^{HF} \Omega_{i}^{HF} \right) \Sigma_{i}^{HF} = \left( \begin{array}{c} S_{i}^{HF} \end{array} W_{i}^{HF} \end{array} \right) =
\]

\[
i U \left[ \left( \frac{1}{2} \text{Tr}[C_{ii}] I + C_{ii} \right) + \left( \frac{1}{2} \text{Tr}[F_{ii}] I + F_{ii} \right) \right],
\]

(13)

\[
S_{i}^{HF} = \left( \begin{array}{c} S_{i}^{HF} \end{array} W_{i}^{HF} \end{array} \right) =
\]

\[
i U \left[ \left( \frac{1}{2} \text{Tr}[C_{ii}] I + \frac{1}{2} \text{Tr}[F_{ii}] I + F_{ii} \right) \right].
\]

(14)

Note that in this approximation quantities related to the spectral function $A_{ij}$ decouple from the system of equa-
tions, and the final system of BHF equations reads

\[ \begin{align*}
\frac{i}{\hbar} \frac{\partial}{\partial t} a_i &= -J(a_{i+1} + a_{i-1}) + (U|a_i|^2 + 2iUF^G_{ii})a_i + iU\xi_f a_i^*, \\
\frac{i}{\hbar} \frac{\partial}{\partial t} F^G_{ij} &= -J(F^G_{i+1,j} + F^G_{i-1,j}) + J(F^G_{ij+1} + F^G_{ij-1}) \\
&\quad + \sum_i \Omega_i \xi_i \left( F^H_{ij} - F^H_{ij}^* - \Omega_i \xi_i \right) + 2\xi_i a_i a_j, \\
\frac{i}{\hbar} \frac{\partial}{\partial t} F^F_{ij} &= -J(F^F_{i+1,j} + F^F_{i+1,j}) - J(F^F_{ij+1} + F^F_{ij-1}) \\
&\quad + \sum_i \Omega_i \xi_i \left( F^H_{ij} + F^H_{ij}^* - \Omega_i \xi_i \right) + 2\xi_i a_i a_j.
\end{align*} \]

(15)

We then solve the equations numerically, the results being discussed in detail in section III.

C. Selfconsistent second-order approximation

In the selfconsistent second-order approximation, accounting for collisions and relaxation, the equations are significantly more complicated, and the spectral and statistical parts are coupled, unlike in the BHF approximation. The diagrammatic contributions to the selfenergies in second order are depicted in Fig. 1. Due to the underlying symmetry relations specified in Appendix A we give here only the expressions for the upper-left and upper-right components of the second-order matrix selfenergy \( \gamma_{ij} \) [see Eqs. (10) – (12)],

\[
\begin{align*}
\gamma^G_{ij} &= U^2 F^G_{ij} (4\Lambda_{ij} [F, F^*] + 2\Lambda_{ij} [G, G^*]) \\
&\quad + U^2 \Lambda^G_{ij} (4\Xi_{ij} [F, F^*] + 2\Xi_{ij} [G, G^*]), \\
\gamma^F_{ij} &= U^2 F^F_{ij} (4\Lambda_{ij} [G, G^*] + 2\Lambda_{ij} [F, F^*]) \\
&\quad + U^2 \Lambda^F_{ij} (4\Xi_{ij} [G, G^*] + 2\Xi_{ij} [F, F^*]).
\end{align*}
\]

(16)

Here we introduced the shorthand notations

\[
\begin{align*}
\Lambda_{ij}[f, g](t, t') &= \Lambda^f_{ij}(t, t') F^g_{ij}(t, t') + \Lambda^g_{ij}(t, t') F^f_{ij}(t, t'), \\
\Xi_{ij}[f, g](t, t') &= F^f_{ij}(t, t') F^g_{ij}(t, t') - \frac{1}{4} \Lambda^f_{ij}(t, t') \Lambda^g_{ij}(t, t'),
\end{align*}
\]

(18)

where \( f, g \in \{ G, F, G^*, F^* \} \) and \( A^g \equiv (A^g)^* \). The other two contributions \( \Gamma_{ij} \) and \( \Pi_{ij} \) from Eqs. (10) – (12) are expressed as follows,

\[
\begin{align*}
\Gamma^G_{ij} &= 2iU^2 (2a_i^* a_j^* \Lambda_{ij} [F, G] + a_i^* a_j^* \Lambda_{ij} [G, G] - 2a_i a_j \Lambda_{ij} [F^*, G] - 2a_i a_j^* \Lambda_{ij} [G, G^*] - 2a_i a_j^* \Lambda_{ij} [F, F^*]) \\
&\quad + U^2 (F^G_{ij} (4\Lambda_{ij} [F, F^*] + 2\Lambda_{ij} [G, G^*]) + \Lambda^G_{ij} (4\Xi_{ij} [F, F^*] + 2\Xi_{ij} [G, G^*])), \\
\Gamma^F_{ij} &= 2iU^2 (2a_i^* a_j^* \Lambda_{ij} [F, G] + a_i^* a_j^* \Lambda_{ij} [F, G] - 2a_i a_j \Lambda_{ij} [F^*, G] - 2a_i a_j^* \Lambda_{ij} [G, G^*] - 2a_i a_j^* \Lambda_{ij} [F, F^*]) \\
&\quad + U^2 (F^F_{ij} (4\Lambda_{ij} [G, G^*] + 2\Lambda_{ij} [F, F^*]) + \Lambda^F_{ij} (4\Xi_{ij} [G, G^*] + 2\Xi_{ij} [F, F^*])),
\end{align*}
\]

(19)

\[
\begin{align*}
\Pi^G_{ij} &= 2iU^2 (2a_i^* a_j^* \Xi_{ij} [F, G] + a_i^* a_j^* \Xi_{ij} [G, G] - 2a_i a_j \Xi_{ij} [F^*, G] - 2a_i a_j^* \Xi_{ij} [G, G^*] - 2a_i a_j^* \Xi_{ij} [F, F^*]) \\
&\quad + U^2 (F^G_{ij} (4\Xi_{ij} [F, F^*] + 2\Xi_{ij} [G, G^*]) - \frac{1}{2} \Lambda^G_{ij} (2\Lambda_{ij} [F, F^*] + \Lambda_{ij} [G, G^*])), \\
\Pi^F_{ij} &= 2iU^2 (2a_i^* a_j^* \Xi_{ij} [F, G] + a_i^* a_j^* \Xi_{ij} [F, G] - 2a_i a_j \Xi_{ij} [F^*, G] - 2a_i a_j^* \Xi_{ij} [G, G^*] - 2a_i a_j^* \Xi_{ij} [F, F^*]) \\
&\quad + U^2 (F^F_{ij} (4\Xi_{ij} [G, G^*] + 2\Xi_{ij} [F, F^*]) - \frac{1}{2} \Lambda^F_{ij} (2\Lambda_{ij} [G, G^*] + \Lambda_{ij} [F, F^*])).
\end{align*}
\]

(20)

(21)

(22)

With these selfenergies, the equations of motion for the spectral and for the statistical functions become, respectively,
\[ i \frac{\partial F_{ij}^G}{\partial t} = -J(F_{i+1,j}^G + F_{i-1,j}^G) + \sum_i H^F F_{ij}^G - \Omega_i^H (F_{ij}^F)^* - i \sum_k \int_0^t d\tau (\Gamma_{ik}^G F_{kj}^G + \Gamma_{ik}^F F_{kj}^F) + i \sum_k \int_0^{t'} d\tau (\Pi_{ik}^G A_{kj}^G + \Pi_{ik}^F A_{kj}^F), \]

\[ i \frac{\partial F_{ij}^F}{\partial t} = -J(F_{i+1,j}^F + F_{i-1,j}^F) + \sum_i H^F F_{ij}^F - \Omega_i^H (F_{ij}^G)^* - i \sum_k \int_0^t d\tau (\Gamma_{ik}^G F_{kj}^G + \Gamma_{ik}^F F_{kj}^F) + i \sum_k \int_0^{t'} d\tau (\Pi_{ik}^G A_{kj}^G + \Pi_{ik}^F A_{kj}^F). \]

(26)

Here, \( t \) refers again to the first time argument of the entities and \( t' \) to the second one. For the notation in the convolution integrals in these equations see the end of section IIA. The sets of equations (23), (24) and (25), (26) are coupled to the equations for the condensate amplitudes on sites \( i \),

\[ i \frac{\partial a_i}{\partial t} = -J(a_{i+1} + a_{i-1}) + (U|a_i|^2 + 2iUF_{ii}^G)a_i + iUF_{ii}^Fa_i^* - i \sum_k \int_0^t d\tau (\gamma_{ik}^G a_k + \gamma_{ik}^F a_k^*). \]

(27)

Note that the integrals in Eqs (23)–(26) still contain \( \overline{G} \) and \( \overline{F} \)-components of spectral and statistical functions. The treatment of such integrals using the symmetry relations from Appendix A is described in detail in Appendix B.

III. RESULTS

We consider a square optical lattice of size \( I \times I \), where \( I \) is the odd number of sites along the \( x \) or \( y \) direction. Each site is addressed by the double index \( i \equiv (n_x, n_y) \) where \( n_x, n_y \) run from \(-(I-1)/2\) to \((I-1)/2\), and summation over \( i \) implies summing over all lattice sites. We will impose periodic boundary conditions, and define the first Brillouin zone such that the quasimomenta \( k_x, k_y \in [0, 2\pi/a] \), where \( a \) is the lattice constant (see also Figs. 2 and 3). The filling factor is \( \rho = N/I^2 \), where \( N \) is the total particle number,

\[ N = \sum_i N_i^0(t) + N_i^c(t) = \sum_i \left[ |a_i(t)|^2 + iF_{ii}^G(t, t) \frac{1}{2} \right]. \]

(28)

In Eq. (28), \( N_i^0(t) \) is the number of condensed particles, while \( N_i^c(t) \) is the particle number in the incoherent
cloud, or fluctuation particle number. The total particle number \( N \) is conserved. This is obeyed by our conserving approximations (the BHF and the 2nd-order selfconsistent approximations). We have also confirmed it in our numerics. We study the expansion dynamics in dependence on the interparticle interaction \( U \), expressed in dimensionless units as

\[ u = \frac{U N}{J} \]  

(29)

and express the time in terms of the dimensionless variable \( J t \).

As the initial condition, we assume that at time \( t = 0 \) all particles are condensed in the central site \((0,0)\) site, that is,

\[ a_i(0) = \sqrt{\rho \gamma} \delta_{i0}, \]
\[ F_{ij}^G(0,0) = -\frac{i}{2} \delta_{ij}, \]
\[ F_{ij}^E(0,0) = 0. \]  

(30)

The temporal expansion of the bosonic gas is then expressed in terms of the time-dependent site occupations \( N_i(t) = N_i^0(t) + N_i^f(t) \), the local fluctuation numbers \( N_i^f(t) \), and \( n_k(t) \), the quasimomentum distribution of the atoms spreading over the optical lattice,

\[ n_k(t) = \frac{1}{T^2} \sum_{i,j} e^{i(k(r_i - r_j))} \left( \langle a_i^*(t) a_j(t) \rangle + \langle b_i^*(t) b_j(t) \rangle \right). \]  

(31)

A. Results without interaction-induced damping

We begin by numerically solving Eqs. \( 15 \) which comprise the BHF approximation. This does not take into account inelastic quasiparticle damping effects, however, it captures many of the salient features of the expansion dynamics, namely, occupation-induced shifts of the single-particle energies, effects of the coherent BEC dynamics including selftrapping, and dynamical creation of the incoherent cloud of single-particle excitations beyond the Gross-Pitaevskii equation (GPE) and its exchange with the BEC.

Fig. 2 shows the dynamical evolution of the condensate expansion for \( I = 21, \rho = 1 \), and \( u = 3 \). The upper row displays the site occupations \( N_i(t)/N \) in real space on a logarithmic scale for different times \( J t \). The expanding cloud reaches the edges of the lattice near \( t J \approx 5 \). Thereafter, the local site occupations re-appear at the respective, opposite sides of the lattice, corresponding to reflection in a finite-size lattice. The interference patterns appearing for times \( J t \geq 5 \) indicate the coherence of the condensate part of the cloud. The fluctuation dynamics is not shown, as the local fluctuations amount to less than 1% of the total population in this case. The fluctuation dynamics will be discussed in detail in Figs. 4 and 5. The second row in Fig. 2 presents the lattice-momentum distribution in the first Brillouin zone for the same times. Throughout the time evolution, the momentum distribution is rather broad, showing interference effects of the condensate again for times \( J t \geq 5 \). It indicates a rather homogeneous expansion of the cloud, with velocities given by \( v_k = \partial \varepsilon_k / \partial k \) and the square lattice.
dispersion $\varepsilon_k = -2J[\cos(k_xa) + \cos(k_ya)]$, as also seen from the real-space pictures.

The expansion dynamics changes drastically when the interaction is increased, as shown in Fig. 3 for $u = 7$. The real-space pictures (first row in Fig. 3) show that the BEC cloud expands more slowly, where the cloud separates in a high-density, central part and a low-density, halo-like structure surrounding it, before the particles get reflected from the boundaries and interference effects set in again. This slow expansion is confirmed by the momentum distribution shown in the second row of Fig. 3. Throughout the time evolution, it remains strongly peaked around $k = (\pi/a, \pi/a)$ where the group velocity of the square lattice vanishes. This behaviour is similar to the experimental observation [4], where for a noninteracting gas a homogenous square spread is observed, whereas for finite interaction a bimodal structure of a slow central cloud surrounded by fast square-shaped background is seen in 2D.

In order to better understand the behaviour of the bimodal structure we plot in Fig. 4 the expansion of the bosonic cloud along the lattice diagonal $n_x = n_y$ versus time for different values of the interaction $u$ and for both, the BEC (upper row) and the incoherent cloud (lower row). While for interaction strength $u \leq 5$ the BEC spreads essentially homogeneously with a slight maximum at the expansion front, the bimodal expansion of the BEC is clearly seen for $u \geq 7$. This can be explained by the selftrapping effect known from bosonic Josephson junctions [18, 19]. It is due to an energy mismatch between neighboring sites, that is, it occurs in the on-linear Gross-Pitaevskii dynamics when the difference between the total condensate energies $u_i = UN_i^0(t)[N_j^0(t) - 1]/(2J)$ on neighboring sites $i, j$, or neighboring potential wells exceeds a critical value [10, 18]. This is fulfilled at the boundaries of the central BEC cloud for $u \geq 7$. As a result, the tunneling of condensate particles from the central, high-density sites to the outer, low-density sites is inhibited, leading to a reduced expansion speed of the central cloud, as seen in Fig. 4, upper row. By contrast, particles on the low-density sites within the halo are not subject to selftrapping and, therefore, propagate outward ballistically with constant, high speed, in agreement with experiment [4]. In fact, as seen from Fig. 4, the halo speed in $x$ direction reaches the Lieb-Robinson limit [20] which for our tight-binding square lattice is $v_{x,\text{max}} = |v_{k=\pi/a}| = 2Ja$. As a result of the different expansion speeds, the central cloud and the halo become spatially separated, leading to a distinct “fore-runner”. This explanation of the bimodal expansion is corroborated by the fact that it is observed only in the expansion of the coherent BEC (upper row), not in the incoherent cloud (lower row of Fig. 4), as expected from the Gross-Pitaevskii dynamics. Rather, the incoherent excitations are dragged along by the coherent, central cloud and their number is unobservably small in the halo for $u \geq 7$. As a remarkable observation, there seems to be an interesting interplay between nonlinear selftrapping and interference for long times. After reflection from the lattice boundaries, the local BEC amplitude may constructively interfere so that locally the selftrapping threshold is reached again, leading to multiple quasilocalized BEC clouds, seen in Fig. 3 upper right panel ($Jt = 15$), as the nine high-occupation regions. They cannot be a mere interference effect, as they are not observed in Fig. 2 for small interaction ($u = 3$).

The role of the incoherent cloud in the expansion dynamics can be analyzed by monitoring the time evol-
The time evolution of the fluctuation energies ( insets of Fig. 6 ) reflects the fluctuation-number dynamics discussed in Fig. 5 . For small interaction ( $u = 3$ ), after the initial, steep increase, the kinetic fluctuation energy $E^{\varphi}_{\text{kin}}(t)$ continues to increase linearly in accordance with the fluctuation number ( Fig. 5 , left panel ), while the interaction energy $E^{\varphi}_{\text{int}}(t)$ settles to a constant value. This shows that, although the overall fluctuation number increases with the volume of the cloud, the fluctuation number on each site remains on a constant, small level.
FIG. 7: Site-resolved expansion in a $3 \times 3$ lattice for $u = 3$ and different filling factors $\rho = 1$, 2, and 3. $N_i^{(0)}(t)$ denotes the condensate number, $N_i^{(\phi)}(t)$ the fluctuation number on site $i$, and $N_i^{(\phi)}(t)$ the total number of fluctuations, each normalized to the total particle number $N$. Black, blue, and orange lines represent the central (0), corner (C), and edge sites (E), respectively, as visualized by the color-coded lattice shown in the inset. The dashed lines correspond to the respective solutions obtained within BHF approximation in all panels.

First, we note that in the small lattice the fluctuation fraction is generally higher than in the large $21 \times 21$ lattice. This may be traced back to the fact that for our initial conditions in the $3 \times 3$ lattice the initial condensate number on the central site is smaller than in the $21 \times 21$ lattice and, thus, fluctuations are less strongly suppressed. For the same reason, selftrapping effects are weaker. Second, for $u = 3$ the time evolution including collisions of incoherent excitations reproduces the BHF approximation for all considered quantities and filling fractions quantitatively rather well (see Fig. 7), as already conjectured at the end of section IIIA. The on-site condensate occupation numbers $N_i^{(0)}(t)$ perform pronounced, weakly damped Josephson-like oscillations [10].

Finally, for $u = 7$ the total local occupation numbers $N_i^{(0)}(t) + N_i^{(\phi)}(t)$ agree again quantitatively well with the BHF approximation, as seen from Fig. 8, first row. However, in this case and for $\rho = 1$, the fraction of fluctuations produced by strong interaction and second-order collisions, deviates strongly from the prediction of the BHF approximation. This leads to fast condensate depletion on all sites, and condensate oscillations are quickly damped, as seen in Fig. 8 (d) and (g). On the other hand, as the filling fraction is increased to $\rho = 2$ and 3, the agreement with the BHF approximation is restored for propagation times of up to $Jt \approx 4$, see Fig. 8 (e)–(f), (h)–(i). Note that these filling fractions correspond to an initial population of the central site of 18 and 27, respectively, which is still far below the initial central-site occupation of $21^2 = 441$ for the $21 \times 21$ lattice.

FIG. 8: Expansion per site in a $3 \times 3$ lattice as in Fig. 7 but for interaction strength $u = 7$.

B. Small lattices with damping

We now investigate the influence of collisions of the incoherent excitations and damping by solving the second-order selfconsistent approximation described by Eqs. 23–27. This requires time-evolving the propagators and selfenergies for two different time arguments. Some details about how to deal with convolution integrals in this case are given in Appendix B. For reasons of numerical costs of computing the second-order selfenergies we only consider a $3 \times 3$ lattice and limited evolution time here. The corresponding results are shown in Figs. 7 and 8 for all the different, inequivalent lattice sites and compared with the BHF results (dashed lines).
at \( \rho = 1 \). Considering that the importance of fluctuations (and, therefore, their interactions) decreases with increasing condensate population, we conclude that the BHF results of section IIIA for a \( 21 \times 21 \) lattice should be reliable at least for the initial time evolution up to \( Jt \approx 5 \), even though quasiparticle collisions are not taken into account there. Consequently, the bimodal expansion separated into a strongly populated central cloud and a weak, quantum coherent halo should be observable, in agreement with the experiment [4].

IV. CONCLUSION

We studied the temporal expansion dynamics of an ultracold Bose gas in the two-dimensional Bose-Hubbard model, where initially all bosons are trapped and condensed at the central site of a square lattice. Within our formalism we are able to analyze separately (1) the semiclassical Gross-Pitaevskii dynamics of the BEC, (2) the dynamics of quantum fluctuations and (3) their inelastic two-body interactions as well as the mutual influence of these components on each other. After a hopping quench, the bosons spread over the lattice in a nontrivial way. We showed that the expansion dynamics depends crucially on interactions. One can clearly distinguish a strongly interacting regime (for our system, \( u \geq 7 \)) when the condensate cloud effectively splits into two parts: a slowly expanding high-density part at the center of the lattice and a fast, quantum coherent, low-density halo or forerunner at the rim of the cloud. This bimodal structure is in qualitative agreement with the experiment [4] and is interpreted as due to nonlinear selftrapping effects. We demonstrated that the velocity of the forerunner is bounded from above by and reaches the maximum group velocity of the system, which represents the Lieb-Robinson limit [20] for this case.

We also showed that in high-density, interacting clouds the quench dynamics leads to an initial, explosive generation of fluctuations, albeit with a small overall amplitude. As the cloud further expands, for weak interaction \( (u = 3, 5) \) the fluctuation number continues to increase, but linearly in time with a moderate slope. For stronger interaction \( (u = 7) \), the role of the condensate as confining potential for the fluctuations starts to dominate, so that the initially created fluctuation numbers are no longer supported by the further expansion dynamics, leading to a peak-like time evolution of the fluctuation number. In this way, the fluctuations remain confined to a low number in high-density systems for all interaction parameters.

For smaller lattices we studied damping effects due to quasiparticle collisions. Since it is numerically a challenging problem, we reduced the analysis to \( 3 \times 3 \) lattices. In this case, the fluctuation numbers are much higher than in larger lattices, as expected. In low-density systems, the collision-induced damping can lead to a fast depletion of the condensate population, transforming the system into an incoherent gas. In the long-time limit, this should lead to a thermal gas [12] above the condensation temperature. For larger filling fractions (or initial central site occupation), however, the coherent BEC dynamics is recovered for significant evolution times. Extrapolating this finding to the large lattice systems, we conclude that the bimodal expansion (see above) should be robust against collisions. This analysis shows the possibly important role of fluctuations, depending on the lattice size and interaction also noted in the experiment [4]. In addition, it provides an explanation why the bimodal expansion (see above) was experimentally observed [4], despite the ubiquitous presence of fluctuations. In the future it will be interesting to study collision effects for disordered as well as periodically driven Bose-Hubbard lattices.

Acknowledgments

We gratefully acknowledge useful discussions with Ulrich Schneider. This work was financially supported by the Deutsche Forschungsgemeinschaft (DFG) within the Cooperative Research Center SFB/TR 185 (Grant No. 277625399) and the Cluster of Excellence MLAQ (Grant No. 390534769).

Appendix A: Symmetry relations

Our equations simplify if we make use of the symmetry relations listed below. For components of spectral function and statistical functions it holds

\[ A_{ij}^F(t,t') = -A_{ij}^G(t,t')^* = -A_{ji}^G(t',t) \]
\[ A_{ij}^F(t,t') = -A_{ij}^F(t,t')^* = A_{ji}^F(t',t) \]
\[ F_{ij}^G(t,t') = -F_{ij}^G(t,t')^* = F_{ji}^G(t',t) \]
\[ F_{ij}^F(t,t') = -F_{ij}^F(t,t')^* = -F_{ji}^F(t',t) \]

The selfenergies which enter Eqs. (10)–(12) also obey the symmetry relations

\[ \gamma_{ij}^G(t,t')^* = -\gamma_{ij}^G(t',t) = \gamma_{ij}^C(t,t') \]
\[ \gamma_{ij}^F(t,t')^* = -\gamma_{ij}^F(t',t) = \gamma_{ij}^F(t',t) \]
\[ \Gamma_{ij}^F(t,t')^* = -\Gamma_{ij}^F(t',t) = \Gamma_{ji}^F(t',t) \]
\[ \Pi_{ij}^F(t,t')^* = -\Pi_{ij}^F(t',t) = -\Pi_{ji}^F(t',t) \]
\[ \Pi_{ij}^G(t,t')^* = -\Pi_{ij}^G(t',t) = -\Pi_{ji}^G(t',t) \]

Appendix B: Convolution integrals in equations of motion

We can use the symmetry relations listed in Appendix A also in the convolution integrals which enter our equa-

[...]

\[ A_{ij}^F(t,t') = -A_{ij}^F(t,t')^* = A_{ji}^F(t',t) \]
We proceed in an analogous way for the other integrals of Eqs. (23)–(26) and then solve the final system of equations numerically.

\[ -i \sum_k \int_0^t dt \left[ \Gamma^G_{ik}(t, \bar{t}) F^{G}_{kj}(\bar{t}, t') + \Gamma^F_{ik}(t, \bar{t}) F^{F}_{kj}(\bar{t}, t') \right] = i \sum_k \int_0^{t'} dt' \left[ \Gamma^G_{ik}(t, \bar{t}) F^{G}_{kj}(\bar{t}, t') + \Gamma^F_{ik}(t, \bar{t}) F^{F}_{kj}(\bar{t}, t') \right]. \]  

(B1)

The symmetry relations allow us to split the interval of integration in such a way that we can rewrite the integrals with the arguments corresponding to the later time as first arguments. Hence, we get for the integral (B1) 

\[ i \sum_k \int_0^{t'} dt' \left[ \Gamma^G_{ik}(t, \bar{t}) F^{G}_{kj}(t', \bar{t}) + \Gamma^F_{ik}(t, \bar{t}) F^{F}_{kj}(t', \bar{t}) \right] + i \sum_k \int_0^{t} dt \left[ \Gamma^G_{ik}(t, \bar{t}) F^{G}_{kj}(t, \bar{t}) + \Gamma^F_{ik}(t, \bar{t}) F^{F}_{kj}(t, \bar{t}) \right]. \]  

(B2)

We proceed in an analogous way for the other integrals of Eqs. (23)–(26) and then solve the final system of equations numerically.