Nonequilibrium Dynamics of Optical Lattice-Loaded BEC Atoms: 
Beyond HFB Approximation

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Abstract

In this work a two-particle irreducible (2PI) closed-time-path (CTP) effective action is used to describe the nonequilibrium dynamics of a Bose Einstein condensate (BEC) selectively loaded into every third site of a one-dimensional optical lattice. The motivation of this work is the recent experimental realization of this system at National Institute of Standards and Technology (NIST) where the placement of atoms in an optical lattice is controlled by using an intermediate superlattice. This patterned loading method is a useful technique for the proposed implementation of lattice-based AMO quantum computing. This system also serves to illustrate many basic issues in nonequilibrium quantum field theory pertaining to the dynamics of quantum correlations and fluctuations which goes beyond the capability of a mean field theory. By numerically evolving in time the initial state configuration using the Bose-Hubbard Hamiltonian an exact quantum solution is available for this system in the case of few atoms and wells. One can also use it to test out the various approximation methods constructed. Under the 2PI CTP scheme with this initial configuration, three different approximations are considered: a) the Hartree-Fock-Bogoliubov (HFB) approximation, b) the next-to-leading order 1/\(N\) expansion of the 2PI effective action up to second order in the interaction strength and c) a second order perturbative expansion in the interaction strength. We present detailed comparisons between these approximations and determine their range of validity by contrasting them with the exact many body solution for a moderate number of atoms and wells. As a general feature we observe that because the second order 2PI approximations include multi-particle scattering in a systematic way, they are able to capture damping effects exhibited in the exact solution that a mean field collisionless approach fails to produce. While the second order approximations show a clear improvement over the HFB approximation our numerical result shows that they do not work so well at late times, when interaction effects are significant.

1 Description of the Problem

Bose-Einstein condensate (BEC) loaded into an optical lattice has provided an interesting arena for the study of quantum coherence and fluctuation phenomena in many body physics. Spectacular progress in experimental studies have been able to achieve regimes where standard mean field techniques used to describe weakly interacting atoms are not generally applicable. The description of the evolution of condensates far from equilibrium has also gained considerable importance in matter-wave physics, motivated by recent experimental realization of colliding and collapsing condensates. In this paper we want to investigate the dynamics of a Bose-Einstein
condensate at zero-temperature (T=0) loaded every three sites in a one dimensional optical lattice, recently realized by the NIST group [1].

In that experiment a combination of two independently controlled lattices was used to prepare the condensate into every third site of a single lattice. Briefly the procedure consists of loading a condensate into the ground band of a lattice with periodicity 3a, so that the condensate is well localized in the potential minima of this lattice. A second lattice of periodicity a which is parallel to the first lattice is then ramped up so that the superimposed light potentials form a super-lattice of period 3a. If both lattices are in phase, then the addition of the new lattice will not shift the locations of the potential minima from those of the first lattice alone and the condensate will remain localized at these positions. Finally, by removing the first period 3a lattice on a time scale long compared to band excitations, but short compared to the characteristic time of dynamics within the lattice, the condensate will be left in every third site of the period a lattice.

A condensate loaded in this way is not an eigenstate of the final period a lattice, and the condensate will continue to evolve in the final system. Outside the strongly correlated regime, a mean field approach was expected to give a good description of the condensate dynamics [2]. However, by comparison with numerical simulations of the exact solution of the many-body Hamiltonian it was found that even in the case when the kinetic energy is comparable with the on-site interactions, inter-atomic collisions play a crucial role in determining the quantum dynamics of the system and therefore a mean field collisionless approach is only accurate for short times.

Thus, in order to model the correct quantum dynamics of the system it is necessary to include properly scattering processes among particles. This task, however, is not easy for this particular system because contrary to the three dimensional dilute gas case, where many body effects introduce only a small change to the two-particle scattering properties in vacuum, the presence of the lattice and the low dimensionality of the system make the problem much less straightforward.

To date most theoretical descriptions of nonequilibrium dynamics are based on the time dependent Gross-Pitaevskii equation coupled with extended kinetic theories that describe excitations near thermal equilibrium situations. These approaches usually rely on the contact-potential approximation of the binary interactions which restricts two-body collisions to low energy. However, system dynamics of most interest falls outside of this restricted domain; its description thus requiring new methods. Here to describe the far-from-equilibrium dynamics we adopt a CTP (Closed Time Path) [3] functional-integral formalism together with a 2PI (two-particle irreducible) [4] effective action approach to derive the equations of motion. This method has been generalized for and applied to the establishment of a quantum kinetic field theory [3] [5] [7] with applications to problems in gravitation and cosmology [3] [8], particles and fields [10] [11], BEC [12] [13] and condensed matter systems [14] as well as addressing the issues of thermalization and quantum phase transitions [15] [16] [17].

In Section 2 we summarize the mean field results obtained in previous studies [2]. In Section 3 we introduce the 2PI generating functional to construct the 2PI effective action $\Gamma_2$ and Green’s functions. In Section 4 we perform perturbative expansions on $\Gamma_2$ and define the various approximation schemes. In Section 5 we introduce the CTP formalism. We then derive the equation of motion and discuss the results under each approximation scheme, starting with HFB in Section 6, followed by second order expansions in Section 7, which includes the $1/N$ expansion and the full second order expansion. The numerical implementation is discussed in Section 8. In Section 9 we present our results and determine the range of validity of the approximations by comparisons with the exact (numerical) solution. We end with the conclusions.

2 Mean Field Theory

The dynamics of an ultracold bosonic gas in an optical lattice can be described by a Bose-Hubbard model where the system parameters are controlled by laser light. For a one dimensional lattice the starting Hamiltonian is:

$$\hat{H} = -J \sum_i (\hat{\Phi}_i^\dagger \hat{\Phi}_{i+1} + \hat{\Phi}_{i+1}^\dagger \hat{\Phi}_i) + \sum_i \epsilon_i \hat{\Phi}_i^\dagger \hat{\Phi}_i + \frac{1}{2} U \sum_i \hat{\Phi}_i^\dagger \hat{\Phi}_i \hat{\Phi}_i \hat{\Phi}_i^\dagger ,$$

(1)
where $\hat{\Phi}_i$ and $\hat{\Phi}_i^\dagger$ are the annihilation and creation operators at the site $i$ which obey the canonical commutation relations for bosons. Here, the parameter $U$ denotes the strength of the on-site repulsion of two atoms on the site $i$; the parameter $\varepsilon_i$ denotes the energy offset of each lattice site due to an additional slow varying external potential such as a magnetic trap and $J$ denotes the hopping rate between adjacent sites. Because the next-to-nearest neighbor amplitudes are typically two orders of magnitude smaller, tunneling to them can be neglected. The Bose-Hubbard Hamiltonian should be an appropriate model when the loading process produces atoms in the lowest vibrational state of each well, with a chemical potential smaller than the distance of the first vibrationally excited state. This is the case of the experiment we want to study.

Here we consider only a one-dimensional homogeneous lattice with periodic boundary conditions. The transverse degrees of freedom and the harmonic confinement in the direction of the lattice are relegated to a future work.

In the simplest version of the mean-field theory, we assume that all atoms share the same condensate wave function and therefore it is possible to replace the operator on the lattice site $i$ by a c-number $\phi_i(t)$. Under this approximation $\phi_i(t)$ corresponds to the time dependent mean value amplitude of the $i^{th}$ well. One might expect that this zero temperature mean field approach could give a good description of the dynamics of the atoms in the limit that quantum fluctuations can be completely neglected, that is, the regime when the ratio $U$ to $J$ is sufficiently small and the tunneling overwhelms the repulsion.

By making the mean field ansatz in the Bose-Hubbard Hamiltonian it is possible to show that the $\phi_i(t)$ amplitudes satisfy the Discrete Non Linear Schrodinger Equation (DNLSE), which in the case of zero external potential has the form:

$$i \frac{\partial \phi_i}{\partial \tau} = - (\phi_{i-1} + \phi_{i+1}) + \frac{UN}{J} |\phi_i|^2 \phi_i,$$

where we have assumed that the $\phi_i(\tau)$ are normalized to one, that $N$ is the total number of atoms and defined a new time scaled $\tau \equiv \frac{\gamma t}{\hbar}$.

We treat a model case in which the initial occupancies of each third site are the same, and in which the condensate initially has a uniform phase. Thus at $t = 0$, the amplitudes $\phi_i(\tau)$ are given by $\phi_{3i}(0) = \sqrt{I/3}$, $\phi_{3i+1}(0) = \phi_{3i+2}(0) = 0$, where $I$ is the total number of lattice sites. For an infinite lattice, or one with periodic boundary conditions, the amplitudes for all initially occupied sites $\phi_{3i}$ evolve identically in time, and the amplitudes for the initially unoccupied sites satisfy $\phi_{3i+1}(\tau) = \phi_{3i+2}(\tau)$ for all $\tau$. This allows us to reduce the full set of equations to a set of two coupled equations for $\phi_0(\tau)$ and $\phi_1(\tau)$.

The solutions $|\phi_0(\tau)|$ and $|\phi_1(\tau)|$ are oscillatory functions whose amplitudes and common period, $T(\gamma)$, are determined by the parameter $\gamma \equiv NUI/(3J)$. It is useful to qualitatively divide the dynamical behavior into two regimes.

**The tunneling dominated regime** ($\gamma < 1$): In this regime we find that the oscillation period is essentially constant, the role of interactions is relatively small, and the equations of motion are equivalent to those of a two-state Rabi problem. This system will undergo Rabi oscillations whereby atoms periodically tunnel from the initially occupied site into the two neighboring sites. For $\gamma = 0$ the period of oscillation is $\frac{2\pi}{\sqrt{3}}$.

**Interaction dominated regime**: The effect of interactions on the mean-field dynamics is to cause the energies of the initially occupied sites to shift relative to those of the unoccupied sites. As $\gamma$ increases the tunneling between sites occurs at a higher frequency, but with reduced amplitude. The population of the initially occupied sites becomes effectively self-trapped by the purely repulsive pair interaction.

To check the validity of the mean field approximation, we made comparisons with the exact many body solution for 6 atoms and three wells. We use a modest number of atoms and lattice sites for the comparisons due to the fact that the Hilbert space needed for the calculations increases rapidly with the number of atoms and wells. The exact solution was obtained by evolving an initial state $e^{-N/2} e^{\sqrt{N}\hat{\Phi}_i^\dagger}|0\rangle \otimes |0\rangle \otimes |0\rangle$ with the
Bose-Hubbard Hamiltonian. The initial state represents just a coherent state with an average of $N$ atoms in the initial populated well. (See Sec. 8.1).

In Fig. 1 we plot the average population per well $\langle \hat{\Phi}^\dagger_i(t) \hat{\Phi}_i(t) \rangle$ and the condensate population per well $\left| \langle \hat{\Phi}_i(t) \rangle \right|^2$ and compare them with the mean field predictions, i.e. $|\phi_i(t)|^2$, for three different values of $\gamma$. The salient features observed in these comparisons are:

**Weakly interacting regime** ($\gamma = 0.2$): The DNLSE gives a good description of the early time dynamics. The total population per well predicted by the mean field solution agrees with the exact solution. This is because the total condensate population remains big for the time in consideration.

**Intermediate regime** ($\gamma = 2$): Quantum fluctuations lead to a non-trivial modulation of the classical oscillations. In this regime the ratio between interaction and kinetic energy is small enough to allow the atoms to tunnel but not too small to make interaction effects negligible, the mean field results are accurate only for a short time. The exact solution exhibits for this regime damped oscillations of the atomic population per well that drives the system towards equilibrium. There is also a very rapid reduction of the condensate population. These characteristic damping effects are caused by the different phase evolution of the quantum states that span the configuration space and collisions among atoms. Quantum scattering effects are crucial, even for rather early times.

**Strongly correlated regime** ($\gamma = 12$): the system exhibits macroscopic quantum self-trapping of the population. Qualitatively, both the mean field and the exact solutions, agree in the sense that atoms are in both self-trapped in the initially populated wells due to interactions. However, the fast decrease of the condensate population and its subsequent revivals shown in the exact solutions give us an idea of the importance of correlation effects beyond mean field in this interaction dominated regime. Due to the fact that the evolution of the initially unoccupied wells is almost frozen by interactions, the collapse and revival of the condensate population can be mainly described by the time evolution of the $n$-particle number states that expand the coherent state of the initially populated well.

Because our main interest is the tunneling dynamics we will focus on the intermediate regime, where the ratio $U/J$ is small but interaction effects are not negligible. In this regime a perturbative expansion around $U/J$ still makes sense.

# 3 2PI Effective Action $\Gamma(\phi, G)$

The first requirement for the study of nonequilibrium processes is a general initial-value formulation depicting the dynamics of interacting quantum fields. The CTP or Schwinger-Keldysh effective action formalism [3] serves this purpose. The second requirement is to describe the evolution of the correlation functions and the mean field on an equal footing. The two particle irreducible (2PI) formalism [4] where the correlation functions appear also as independent variables serves this purpose. By requiring the generalized (master) CTP effective action [4] to be stationary with respect to variations of the correlation functions an infinite set of coupled (Schwinger-Dyson) equations for the correlation functions is obtained which is a quantum analog of the BBGKY hierarchy. The 2PI effective action produces two such functions in this hierarchy. In this section we shall focus on the 2PI formalism, and then upgrade it to the CTP version in the next section.

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1 The partial revival of the condensate population can be understood as the interference of states approximated by a quadratic spectrum: $E_n \approx U/2n(n - 1)$. At first, the different phase evolution of the $n$-particle states leads to a collapse of the condensate population. However at integer values of $t_{rev} = (U/h)^{-1}$ the phase factors add to an integer value of $2\pi$, leading to a revival of the initial state [15]. The revival is not complete because $J$ is not exactly zero. The collapse time $t_c$ depends on the variance of the initial atomic distribution $t_c \approx (t_{rev}/\sigma)$ (See Ref. [19]-[20]). For the initial Poissonian distribution $t_c \approx (U\sqrt{N}/h)^{-1}$. 

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An adequate description of the dynamics of atoms loaded into an optical lattice is provided by the Bose-Hubbard Hamiltonian \( H \), whose classical action is given in terms of the complex fields \( \Phi_i \) and \( \Phi_i^* \) by

\[
S[\Phi_i^*, \Phi_i] = \int dt \sum_i \frac{i\hbar}{2} \Phi_i^*(t) \partial_t \Phi_i(t) + J (\Phi_i^*(t) \Phi_{i+1}(t) + \Phi_i(t) \Phi_{i+1}^*(t)) - \frac{U}{2} \Phi_i^*(t) \Phi_i(t) \Phi_i(t),
\]

where, as before, \( i \) denotes the lattice position, \( J \) is the hopping rate and \( U \) is the interaction strength. We limit the analysis to the case when no external potential is present and include only nearest neighbor hopping.

To compactify our notation we introduce \( \Phi_i^a(a = 1, 2) \) defined by

\[
\Phi_i = \Phi_i^1, \quad \Phi_i^* = \Phi_i^2.
\]

In terms of these fields the classical action takes the form

\[
S[\Phi] = \int dt \sum_i \frac{1}{2} \hbar \partial_t \Phi_i(t) \Phi_i(t) + J \sigma_{ab} \Phi_i^a(t) \Phi_i^b(t) + \frac{U}{4N} (\sigma_{ab} \Phi_i^a(t) \Phi_i^b(t))^2,
\]

where \( N \) is the number of fields, which is two in this case, and summation over repeated field indices \( a, b = (1, 2) \) is implied. \( h_{ab} \) and \( \sigma_{ab} \) are matrices defined as

\[
h_{ab} = i \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad \sigma_{ab} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

After second quantization the fields \( \Phi_i^a \) are promoted to operators. We denote the expectation value of the field operator or mean field by \( \phi_i^a(t) \) and the expectation value of the composite field by \( G_{ij}(t, t') \). Physically, \( |\phi_i^a(t)|^2 \) is the condensate population and the composite fields determine the fluctuations around the mean field.

\[
\phi_i^a(t) = \langle \Phi_i^a(t) \rangle, \quad hG_{ij}(t, t') = \langle T_C \Phi_i^a(t) \Phi_j^b(t') \rangle - \langle \Phi_i^a(t) \rangle \langle \Phi_j^b(t') \rangle.
\]

The brackets denote taking the expectation value respect to the density matrix and \( T_C \) denotes time ordering along a contour \( C \) in the complex plane.

All correlation functions of the quantum theory can be obtained from the effective action \( \Gamma[\phi, G] \), the two particle irreducible generating functional for Green’s functions parametrized by \( \phi_i^a(t) \) and the composite field \( G_{ij}(t, t') \). To get an expression for the effective action we first define the functional \( Z[J, K] \) as

\[
Z[J, K] = e^{iW[J, K]} = \prod_a \int D\Phi^a \exp \left\{ \frac{i}{\hbar} \left[ S[\Phi] + \int dt \sum_i J_{ia}(t) \Phi_i^a(t) + \frac{1}{2} \int dt dt' \sum_{ij} \Phi_i^a(t) \Phi_j^b(t') K_{ijab}(t, t') \right] \right\},
\]

where we have introduced the following index lowering convention

\[
X_a = \sigma_{ab} X^b.
\]
We define $\Gamma[\phi, G]$ as the double Legendre transform of $W[J, K]$ such that

$$\frac{\delta W[J, K]}{\delta J_{ia}(t)} = \phi^a_i(t),$$

$$\frac{\delta W[J, K]}{\delta K_{ijab}(t, t')} = \frac{1}{2} \phi^a_i(t)\phi^b_j(t') + \hbar G^{ab}_{ij}(t, t').$$

Expressing $J$ and $K$ in terms of $\phi$ and $G$

$$\Gamma[\phi, G] = W[J, K] - \int dt \sum_i J_{ia}(t)\phi^a_i(t) - \frac{1}{2} \int dt dt' \sum_{ij} \phi^a_i(t)\phi^b_j(t')K_{ijab}(t, t').$$

From this equation the following identity can be derived:

$$\frac{\delta \Gamma[\phi, G]}{\delta \phi^a_i(t)} = -\left( J_{ia}(t) + \int dt' \sum_j (K_{ijad}(t, t'))\phi^d_j(t') \right),$$

$$\frac{\delta \Gamma[\phi, G]}{\delta G^{ab}_{ij}(t, t')} = -\frac{\hbar}{2} K_{ijab}(t, t').$$

In order to get an expression for $\Gamma[\phi, G]$ notice that by using Eq. (9) for $W[J, K]$ and placing it in Eq. (14) for $\Gamma[\phi, G]$, it can be written as

$$\exp\left(\frac{i}{\hbar} \Gamma[\phi, G]\right) = \prod_a \int D\Phi^a \exp\left\{ \frac{i}{\hbar} \left( S[\Phi] + \int dt_i J_{ia}(t) [\Phi^a_i(t) - \phi^a_i(t)] \\
+ \frac{1}{2} \int dt_i dt'_j \left( \Phi^a_i(t)K_{ijab}(t, t')\Phi^b_j(t') - \phi^a_i(t)K_{ijab}(t, t')\phi^b_j(t') \right) - \frac{\hbar}{2} \text{Tr}GK \right) \right\}$$

$$= \prod_a \int D\Phi^a \exp\left\{ \frac{i}{\hbar} \left( S[\Phi] - \int dt_i \delta\Gamma[\phi, G]_{\phi^a_i(t)} [\Phi^a_i(t) - \phi^a_i(t)] \right) \\
- \frac{1}{\hbar} \int dt_i dt'_j \left[ \Phi^a_i(t) - \phi^a_i(t) \right] \delta\Gamma[\phi, G]_{\phi^b_j(t)} [\Phi^b_j(t') - \phi^b_j(t')] + \text{Tr}G\delta\Gamma[\phi, G]_{\phi^a_i(t)\phi^b_j(t')} \right\},$$

where $\text{Tr}$ means taking the trace. For simplicity we have denoted $\int dt \sum_i$ by $\int dt_i$. Defining the fluctuation field, $\varphi^a_i = \Phi^a_i - \phi^a_i$, we have

$$\Gamma[\phi, G] - \text{Tr}G\delta\Gamma[\phi, G]_{\phi^a_i(t)} = -i\hbar \ln \prod_a \int D\varphi^a \exp\left( \frac{i}{\hbar} S[\phi, G; \varphi] \right)$$

$$S[\phi, G; \varphi] = S[\phi + \varphi] - \int dt_i \delta\Gamma[\phi, G]_{\phi^a_i(t)} \varphi^a_i(t) - \frac{1}{\hbar} \int dt_i dt'_j \varphi^a_i(t) \delta\Gamma[\phi, G]_{\phi^b_j(t')} \varphi^b_j(t').$$

By introducing the classical inverse propagator $iD^{-1}(\phi)$ given by
the solution of the functional integro-differential equation (17) can be expressed as

\[ S \text{ determined by the interaction terms in } \]

setting the right hand side equal to zero. This procedure leads to the following equations:

the mean field and the propagators are found by using the expression (20) in equations (14) and (15), and become disconnected by cutting two propagator lines) in the theory with propagators set equal to \( \Sigma \) it consists of all two-particle irreducible vacuum graphs (the diagrams representing these interactions do not become disconnected by cutting two propagator lines) in the theory with propagators set equal to \( G \) and vertices determined by the interaction terms in \( S[\phi + \varphi] \).

Since physical processes correspond to vanishing sources \( J \) and \( K \), the dynamical equations of motion for the mean field and the propagators are found by using the expression \[ \Gamma[\phi, G] = S[\phi] + \frac{i}{2} Tr \ln G^{-1} + \frac{i}{2} Tr D^{-1}(\phi) G + \Gamma_2[\phi, G] + \text{const.} \] in equations (14) and (15), and setting the right hand side equal to zero. This procedure leads to the following equations:

\[ h_{ab} \partial_t \phi_i^a(t) = -J(\phi_{i+1a}(t) + \phi_{i-1a}(t)) + \frac{U}{N}(\phi_{id}(t)\phi_i^d(t) + G_{ic}(t, t))\phi_{ia}(t) + \]

\[ \frac{U}{N}((G_{iad}(t, t) + G_{ida}(t, t))\phi_i^d(t) - \frac{\delta \Gamma_2[\phi, G]}{\delta \phi_i^a(t)}), \]

and

\[ G^{-1}_{ijab}(t, t') = D_{ijab}(t, t')^{-1} - \Sigma_{ijab}(t, t'), \]

\[ \Sigma_{ijab}(t, t') = 2i \frac{\delta \Gamma_2[\phi, G]}{\delta G_{ij}^a(t', t')} \]

Equation (24) can be rewritten as a partial differential equation suitable for initial value problems by convolution with \( G \). This differential equation reads explicitly

\[ h^a \partial_t G^{ab}_{ij}(t, t') = -J(G_{i+1j}^{ab}(t, t') + G_{i-1j}^{ab}(t, t')) + \frac{U}{N}(\phi_{id}(t)\phi_i^d(t))G^{ab}_{ij}(t, t') + \]

\[ \frac{2U}{N} \phi_i^a(t)G^{ab}_{ij}(t, t')\phi_{ic}(t) + i \int dt'' \Sigma_{ijab}^{ac}(t, t'')G^{ab}_{kj}(t'', t') + i \delta^{ab} \delta_{ij} \delta(t - t'). \]

The evolution of \( \phi^a \) and \( G^{ab} \) is determined by Eqs. (22) and (25) once \( \Gamma_2[\phi, G] \) is specified.
4 Perturbative Expansion of $\Gamma_2(\phi, G)$ and Approximation Schemes

The diagrammatic expansion of $\Gamma_2$ is illustrated in Fig. 2, where two and three-loop vacuum diagrams are shown. The dots where four lines meet represent interaction vertices. The expression corresponding to each vacuum diagram should be multiplied by a factor $(-i)^l (i)^{s-2}$ where $l$ is the number of solid lines and $s$ the number of loops the diagram contains.

The action $\Gamma$ including the full diagrammatic series for $\Gamma_2$ gives the full dynamics. It is of course not feasible to obtain an exact expression for $\Gamma_2$ in a closed form. Various approximations for the full 2PI effective action can be obtained by truncating the diagrammatic expansion for $\Gamma_2$. Which approximation is most appropriate depends on the physical problem under consideration:

4.1 The standard approaches

1. Bogoliubov (One-loop) Approximation:
   The simplest approximation consists of discarding $\Gamma_2$ altogether. This yields the so called Bogoliubov or one-loop approximation whose limitations have been extensively documented in the literature (21, 22).

2. Time-dependent Hartree-Fock-Bogoliubov (HFB) Approximation:
   A truncation of $\Gamma_2$ retaining only the first order diagram in $U$, i.e., keeping only the double-bubble diagram, Fig. 2a, yields equations of motion of $\phi$ and $G$ which correspond to the time dependent Hartree-Fock-Bogoliubov (HFB) approximation. This approximation violates Goldstone’s theorem, but conserves energy and particle number (23, 24, 25). The HFB equations can also be obtained by using cumulant expansions up to the second order in which all cumulants containing three or four field operators are neglected. The HFB approximation neglects multiple scattering. It can be interpreted as an expansion in terms of $Ut/J$, (where $t$ is the time of evolution) and is good for the description of short time dynamics or weak interaction strengths. It will be described in Sec. 6.

4.2 Higher order expansions

We make a few remarks on the general properties of higher order expansions and then specialize to two approximations.

2PI and Ladder Diagrams Since the work of Beliaev’s (29) and Popov (30) it is well known in the literature (see for example Ref. (12, 31)) that including higher order terms in a diagrammatic expansion corresponds to renormalizing the bare interaction potential to the four-point vertex, thus accounting for the repeated scattering of the bosons. In Ref. (32) the authors have shown explicitly for a homogeneous Bose gas that taking into account the two-loop contribution to the 2PI effective action leads to diagrams topologically identical to those found by Beliaev but with the exact propagator instead of the one-loop propagator. In the dilute gas limit, where the inter-particle distance is large compared with the $s$-wave scattering length, the ladder diagrams give the largest contribution to the four-point vertex. Every rung in a ladder contributes to a factor proportional to $Um$ (In the presence of the lattice $m$ should be replaced by the effective mass $m^* (m^* \sim \hbar^2/(Ja^2))$ with $a$ the lattice spacing). The ladder resummation results in an effective potential which is called the $T$- matrix. To lowest order in the diluteness parameter, the $T$-matrix in 3-D systems can be approximated by a constant proportional to $Um$ (pseudopotential approximation). However this approximation is only valid in the weak interaction limit and neglects all momentum dependence which appear in the problem as higher order terms. In that sense the 2PI effective action approach allows us to go beyond the weakly interacting limit in a systematic way and to treat collisions more accurately.
Nonlocal Dissipation and Non-Markovian Dynamics  Higher order terms lead to nonlocal equations and dissipation. The presence of nonlocal terms in the equations of motion is a consequence of the fact that the 2PI effective action really corresponds to a further approximation of the master effective equation. The 2PI effective action is obtained by the slaving of the three point function $C_3$ to the mean field and $G$ with a particular choice of boundary conditions. See Ref. [6] for further details.

Non-Markovian dynamics is a generic feature of the nPI formalism which yields integro-differential equations of motion. This makes numerical solution difficult, but is a necessary price to pay for a fuller account of the quantum dynamics. Many well acknowledged approaches to the quantum kinetics of such systems adopt either explicitly or implicitly (or at the end what amounts to) a Markovian approximation. It assumes that only the current configuration of the system, but not its history, determines its future evolution. Markovian approximations are made if one assumes instantaneous interactions, or in the kinetic theory context that the time scales between the duration of binary collisions $\tau_o$ and the inverse collision rate $\tau_c$ are well-separated. In the low kinetic energy, weak interacting regime the time between collisions (or mean free path) is long compared to the reaction time (or scattering length): $\tau_c >> \tau_o$. The long separation between collisions and the presence of intermediate weak fluctuations, allow for a rapid decay of the temporal and spatial correlations created between collision partners, which one can use to justify the Markovian approximation. However, in the problem at hand, owing to the presence of the lattice which confines the atoms to the bottom of the wells with enhanced interaction effects, the low dimensionality of the system and the far-from-equilibrium initial conditions, non-Markovian dynamics needs to be confronted squarely. That is the rationale for our adoption of the CTP 2PI scheme. Now, for the specifics:

1. Second Order expansion:
   A truncation retaining diagrams of second order in $U$ containing besides the double-bubble, also the setting-sun and the basket-ball Fig.2. By including the setting-sun and the Basket-ball in the approximations we are taking into account two particle scattering processes [9, 7]. Second order terms lead to integro-differential equations which depend on the history of the system.

2. Large-$N$ approximation
   The $1/N$ expansion is a controlled non-perturbative approximation scheme which can be used to study non-equilibrium quantum field dynamics in the regime of strong interactions [16, 15]. In the large $N$ approach the field is modeled by $N$ fields and the quantum field generating functional is expanded in powers of $1/N$. In this sense the method is a controlled expansion in a small parameter but unlike perturbation theory in the coupling constant, which corresponds to an expansion around the vacuum, the large $N$ expansion corresponds to an expansion of the theory about a strong quasiclassical field.

In this work we will derive the equations of motion and perform numerical calculations up to the second order in the coupling constant $U$. This will enable us to determine the range of validity of three types of approximations described above, namely, a) the HFB, b) the full second order and c) NLO large $N$ expansion up to second order in $U$ (in the figures we use the shorthand HFB, 2nd and $1/N$ respectively) by comparison with the exact many body solution for a moderate number of atoms and wells.

5  CTP formalism
In order to describe the non-equilibrium dynamics we will now specify the contour of integration in Eqs. 22 and 25 to be the Schwinger-Keldysh contour along the real-time axis or closed time path (CTP) contour. The Schwinger-Keldysh formalism is a powerful method for deriving real and causal evolution equations for the expectation values of quantum operators for nonequilibrium fields. The basic idea of the CTP formalism relies on the fact that a diagonal matrix element of a system at a given time, $t = 0$ can be expressed as a product of transition matrix elements from $t = 0$ to $t'$ and the time-reverse (complex conjugate) matrix element from
\textit{t}' to 0 by inserting a complete set of states into this matrix element at the later time \textit{t}' . Since each term in the product is a transition matrix element of the usual or time reversed kind, the standard path integral representation for each one can be introduced. However, to get the generating functional we seek, we have to require that the forward time evolution takes place in the presence of a source \textit{J}+ but the reversed time evolution takes place in the presence of a different source \textit{J}−, otherwise all the dependence on the source drops out.

The doubling of sources, the fields and integration contours suggest introducing a 2 x 2 matrix notation. This notation has been discussed extensively in the literature (see [5] [7]). However we are going to follow Refs. [15] and [16] and introduce the CTP formalism in our equation of motion by using the composition rule for transition amplitudes along the time contour in the complex plane. This way is cleaner notationally and has the advantage that all the functional formalism of the previous section may be taken with the only difference of path ordering according to the complex time contour \textit{C}ctp in the time integrations.

The two-point functions are decomposed as

\[
G_{ij}^{\alpha}(t, t') = \theta_{ctp}(t, t')G_{ij}^{\alpha^+}(t, t') + \theta_{ctp}(t', t)G_{ij}^{\alpha^-}(t, t'),
\]

where

\[
hG_{ij}^{\alpha^+}(t, t') = \langle \varphi_i(t)\varphi_j^+(t') \rangle,
\]

\[
hG_{ij}^{\alpha^-}(t, t') = \langle \varphi_i^+(t)\varphi_j(t) \rangle,
\]

with \varphi_i being the fluctuation field and \theta_{ctp}(t−t') being the CTP complex contour ordered theta function defined by

\[
\theta_{ctp}(t, t') = \begin{cases} 
\theta(t, t') & \text{for } t \text{ and } t' \text{ both on } C^+ \\
\theta(t', t) & \text{for } t \text{ and } t' \text{ both on } C^- \\
1 & \text{for } t \text{ on } C^- \text{ and } t' \text{ on } C^+ \\
0 & \text{for } t \text{ on } C^+ \text{ and } t' \text{ on } C^- 
\end{cases}
\]

With these definitions the matrix indices are not required. When integrating over the second half \textit{C}−, we have to multiply by a negative sign to take into account the opposite direction of integration.

To show explicitly that the prescription for the CTP integration explained above does lead to a well-posed initial value problem with causal equations, let us explicitly consider the integral in Eq. (29). The integrand has the CTP ordered form

\[
\Sigma(t, t''\prime)G(t''\prime, t''') = \theta_{ctp}(t, t''\prime)\theta_{ctp}(t''\prime, t'')\Sigma^+(t, t''\prime)G^+(t''\prime, t'') + \theta_{ctp}(t, t''\prime)\theta_{ctp}(t'\prime, t'')\Sigma^+(t, t''\prime)G^-(t''\prime, t'') + \theta_{ctp}(t''\prime, t')\Sigma^-(t, t''\prime)G^+(t''\prime, t') + \theta_{ctp}(t''\prime, t')\theta_{ctp}(t', t'\prime)\Sigma^-(t, t''\prime)G^-(t''\prime, t'),
\]

where we have omitted the indices because they are not relevant for the discussion. Using the rule for CTP contour integration we get

\[
\int dt''\prime\Sigma(t, t''\prime)G(t''\prime, t') = \int_0^t dt'' \theta(t', t'')\Sigma^+(t', t'')G^+(t'', t') + \theta(t', t'')\Sigma^+(t', t'')G^-(t'', t') + \int_t^\infty dt'' \theta(t', t'')\Sigma^+(t', t'')G^+(t'', t') + \theta(t', t'')\Sigma^-(t', t'')G^-(t'', t') - \int_0^\infty dt'' \Sigma^-(t, t'')G^+(t'', t').
\]
If $t > t'$, we have

$$
\int dt'' \Sigma(t, t'')G(t'', t') = \int_0^t dt'' \left( \Sigma^>(t, t'') - \Sigma^<(t, t'') \right) G^>(t'', t') - \int_0^t dt'' \Sigma^>(t, t'')G^>(t'', t') - G^<(t'', t').
$$

(32)

On the other hand, if $t < t'$

$$
\int dt'' \Sigma(t, t'')G(t'', t') = \int_0^t dt'' \left( \Sigma^>(t, t'') - \Sigma^<(t, t'') \right) G^<(t'', t') - \int_0^t dt'' \Sigma^>(t, t'')G^>(t'', t') - G^<(t'', t').
$$

(33)

The above equations are explicitly causal.

It is convenient to express the evolution equations in terms of two independent two-point functions which can be associated to the expectation values of the commutator and the anti-commutator of the fields. We define, following Ref. \[16\] the functions

$$
G_{ij}^{(F)ab}(t, t') = \frac{1}{2} \left( G_{ij}^{ab>}(t, t') + G_{ij}^{ab<}(t, t') \right),
$$

(34)

$$
G_{ij}^{(\rho)ab}(t, t') = i \left( G_{ij}^{ab>}(t, t') - G_{ij}^{ab<}(t, t') \right),
$$

(35)

where the $(F)$ functions are usually called statistical propagators and the $(\rho)$, spectral functions. (See Ref. \[33\].) With these definitions Eq. (23) can be rewritten as:

$$
h^a_\alpha h_\beta \partial_t G_{ij}^{(F)cb}(t, t') = -J \left( G_{ij+1}^{(F)ab}(t, t') + G_{ij-1}^{(F)ab}(t, t') \right) - \frac{2U}{N} \left( \phi_i(t)G_{ij}^{(F)cb}(t, t')\phi_j(t) \right) + \int_0^t dt'' \Sigma_{ik}^{(\rho)ac}(t, t'')G_{kj}^{(F)b}(t'', t') + \int_0^t dt'' \Sigma_{ik}^{(F)ac}(t, t'')G_{kj}^{(\rho)b}(t'', t'),
$$

(36)

$$
h^a_\alpha h_\beta \partial_t G_{ij}^{(\rho)cb}(t, t') = -J \left( G_{ij+1}^{(\rho)ab}(t, t') + G_{ij-1}^{(\rho)ab}(t, t') \right) - \frac{2U}{N} \left( \phi_i(t)G_{ij}^{(\rho)cb}(t, t')\phi_j(t) \right) + \int_0^t dt'' \Sigma_{ik}^{(\rho)ac}(t, t'')G_{kj}^{(\rho)b}(t'', t') + \int_0^t dt'' \Sigma_{ik}^{(\rho)ac}(t, t'')G_{kj}^{(\rho)b}(t'', t'),
$$

(37)

In particular, we define the normal, $\rho$, and anomalous, $m$, spectral and statistical functions as

$$
G_{ij}^{21(F)}(t, t') \equiv \rho_{ij}^{(F)}(t, t') = \frac{1}{2} \left\langle \varphi_i^\dagger(t)\varphi_j(t') + \varphi_j(t')\varphi_i^\dagger(t) \right\rangle,
$$

(38)

$$
G_{ij}^{21(\rho)}(t, t') \equiv \rho_{ij}^{(\rho)}(t, t') = i \left\langle \varphi_i^\dagger(t)\varphi_j(t') - \varphi_j(t')\varphi_i^\dagger(t) \right\rangle,
$$

(39)

$$
G_{ij}^{11(F)}(t, t') \equiv m_{ij}^{(F)}(t, t') = \frac{1}{2} \left\langle \varphi_i(t)\varphi_j(t') + \varphi_j(t')\varphi_i(t) \right\rangle,
$$

(40)

$$
G_{ij}^{11(\rho)}(t, t') \equiv m_{ij}^{(\rho)}(t, t') = i \left\langle \varphi_i(t)\varphi_j(t') - \varphi_j(t')\varphi_i(t) \right\rangle,
$$

(41)

With these relations in place, we now proceed to derive the time evolution equations for the mean field and the two-point functions from the CTP 2PI effective action for the Bose-Hubbard Model under the three approximations described before.
6 HFB Approximation

As remarked in Section 2 the first order mean field approximation leads to a DNLSE which includes only the contribution from the condensate. The HFB equations go beyond the first order approximation and include the leading order contribution of $\Gamma_2$. They describe the coupled dynamics of condensate and non-condensate atoms which arise from the most important scattering processes which are direct, exchange and pair excitations. The basic damping mechanism present in the HFB approximation are Landau and Beliaev damping associated with the decay of an elementary excitation into a pair of excitations in the presence of condensate atoms ([25, 26]). However, these kinds of damping found in the HFB approximation (due to phase mixing, as in the Vlasov equation [27]) are different in nature from the collisional dissipation (as in the Boltzmann equation) responsible for thermalization processes. Multiple scattering processes are neglected in this approximation. We expect the HFB equations to give a good description of the dynamics in the collisionless regime when interparticle collisions play a minor role.

The leading order contribution of $\Gamma_2$ is represented by the double-bubble diagram. Its contribution to $\Gamma_2$ is $\phi$ independent and has an analytic expression of the form

$$\Gamma_2^{(1)}[G] = -\frac{U}{4N} \int dt_i \left( G_{iia}(t,t)G_{iib}(t,t) + 2G_{iab}(t,t)G_{iib}(t,t) \right),$$

the factor of two arises because the direct and exchange terms are identical.

Using the first order expression for $\Gamma_2$ in Eqs. (22) and (25) yields the following equations of motion.

$$\hbar \partial_t \phi_i(t) = -\frac{U}{N} \sum_{j, a} \left( \phi_i a(t) \phi_j^a(t) + G_{iia}(t,t) \phi_j^a(t) \right),$$

$$\hbar \partial_l G_{ij}^{ab}(t,t') = \frac{2U}{N} \left( \phi_i a(t) \phi_j b(t') + G_{iib}(t,t') \phi_j b(t') \right),$$

$$\hbar \partial_t \phi_i(t) = -J\left( \phi_i a(t) \phi_{i-1} b(t) + G_{iia}(t,t) \phi_{i-1} b(t) \right) + \frac{U}{N} \sum_{j, a} \left( \phi_i a(t) \phi_j^a(t) + G_{iia}(t,t) \phi_j^a(t) \right) + \frac{U}{N} \sum_{j, a} \left( \phi_i a(t) \phi_j b(t') + G_{iib}(t,t') \phi_j b(t') \right).$$

In terms of the spectral and statistical functions, Eqs. (28) to (31), and setting $N = 2$, the above equations take the form

$$i\hbar \partial_t \phi_i(t) = -J(\phi_i a(t) \phi_{i-1} b(t)) + U(\phi_i a(t)^2 + 2\rho_i a(t)) \phi_i(t) + U m_i^a(t) \phi_i^a(t),$$

$$-i\hbar \partial_t \rho_i^a(t, t') = L_{ik}(t) \rho_k^a(t, t') + M_{ik}^a(t) m_k^a(t, t'),$$

$$-i\hbar \partial_t \rho_i^b(t, t') = L_{ik}(t) \rho_k^b(t, t') + M_{ik}^b(t) m_k^b(t, t'),$$

$$i\hbar \partial_t m_i^a(t, t') = L_{ik}(t) m_k^a(t, t') + M_{ik}^a(t) \rho_k^a(t, t'),$$

$$i\hbar \partial_t m_i^b(t, t') = L_{ik}(t) m_k^b(t, t') + M_{ik}^b(t) \rho_k^b(t, t').$$

\(^2 \text{We make a distinction between the meaning of the words 'damping' and 'dissipation', the former referring simply to the phenomenological decay of some function, the latter with theoretical meaning, e.g., in the Boltzmann sense.}\)
with

\[ L_{ij}(t) = -J(\delta_{i+1} + \delta_{i-1}) + 2U\delta_{ij} (|\phi_i(t)|^2 + \rho_{ii}^F(t, t)) \tag{50} \]
\[ M_{ij}(t) = U\delta_{ij} (\phi_i(t)^2 + m_{ii}^F(t, t)) \tag{51} \]

The time dependent HFB equations are a closed set of self-consistent equations that describe the coupled dynamics of the condensate and non-condensate components of a Bose gas. It can be checked that they preserve important conservation laws such as the number of particles and energy. The conservation properties of the HFB equations can also be understood by the fact that these equations can also be derived using Gaussian variational methods \[23\]. These methods always yield a classical Hamiltonian dynamics which guarantees probability conservation. Because they are local in time they can be decoupled by a mode decomposition. (See Appendix 1 for details).

7 Second order expansion

7.1 Equations of Motion

7.1.1 Full second order

The second order contribution to \( \Gamma_2 \) is described in terms of the setting-sun Fig. (2b) and the basket-ball Fig. (2c) diagrams. The basket-ball diagram is independent of the mean-field and is constructed with only quartic vertices. The setting-sun diagram depends on \( \phi \) and contains only three-point vertices. The second order \( \Gamma_2^{(2)} \) effective action can be written as

\[
\Gamma_2^{(2)}[\phi, G] = i \left( \frac{U}{2N} \right)^2 \int dt dt' j_{i\alpha}(t) j_{j\beta}(t') \left( G_{ij}^{bb}(t, t') G_{ijdd}(t, t') G_{ijdd}(t, t') + 2G_{ij}^{bd}(t, t') G_{ijdd}(t, t') G_{ij}^{db}(t, t') \right) + i \left( \frac{U}{2N} \right)^2 \int dt dt' j_{i\alpha}(t) j_{j\beta}(t') G_{ijbb}(t, t') G_{ijdd}(t, t') G_{ijdd}(t, t') + 2G_{ijbb}(t, t') G_{ijdd}(t, t') G_{ijdd}(t, t') G_{ij}^{db}(t, t'). \tag{52} \]

To simplify the notation, let us introduce the following definitions \[10\]:

\[
\Pi_{ij}(t, t') = -\frac{1}{2} G_{ijab}(t, t') G_{ijab}(t, t'), \tag{53} \\
\Xi_{ijab}(t, t') = -D(t, t') G_{ijab}(t, t'), \tag{54} \\
D(t, t') = \phi_{a\beta}(t) \phi_{a\alpha}(t') G_{ij}^{ba}(t, t') - \Pi_{ij}(t, t'), \tag{55} \\
\Lambda_{ij}^b(t, t') = -G_{ij}^{bb}(t, t') G_{ijac}(t, t'), \tag{56} \\
\Lambda_{ij}^a(t, t') = -G_{ij}^{ab}(t, t') G_{ijac}(t, t'), \tag{57} \\
\Theta_{ijac}(t, t') = -(\phi_{a\alpha}(t) \phi_{b\beta}(t') + G_{ijdb}(t, t')) G_{ij}^{ab}(t, t') G_{ij}^{dc}(t, t') + \Xi_{ijac}(t, t'). \tag{58} 
\]

With the above definitions we find from Eqs. \[24\] and \[26\] the following equations of motion:
The 2PI effective action is a singlet under $O(N)$ rotations. It can be shown that all graphs contained in an $O(N)$ expansion can be built from the irreducible invariants\[10]: $\phi^2$, $\text{tr}(G^n)$ and $\text{tr}(\phi \phi G^n)$, with $n < N$. The factors of $N$ in a single graph contributing to the same $1/N$ expansion have then two origins: a factor of $N$ from each irreducible invariant and a factor of $1/N$ from each vertex. The leading order large $N$ approximation scales proportional to $N$, the next to leading order (NLO) contributions are of order 1 and so on. At leading order only the first term of Eq. \[12\] contributes. At the next to leading order level, if we truncate up to second order in the coupling strength, the double-bubble is totally included but only certain parts of the setting-sun and basket-ball diagrams are: the first term in both of the integrals of Eq. \[21\],

$$
\Gamma_{2/1+1/N}^{(2)}[\phi, G] = \frac{U}{N} \left( \frac{2}{N} \right)^2 \int dt dt' \phi_{ij}(t) \phi_{ji}'(t') \left( G_{ij}^{bb'}(t, t') \right) G_{ij}^{dd'}(t, t') + \frac{U}{2N} \int dt dt' \phi_{ij}(t) \phi_{ji}'(t') \left( G_{ij}^{bb'}(t, t') \right) G_{ij}^{dd'}(t, t') \right). \tag{60}
$$

The equations of motion under this approximation are the ones obtained for the full second order expansion but with $\Lambda = \Xi = 0$, and $\Theta = \Xi$.

In Appendix 2 we explicitly write the equations of motion in terms of the spectral and statistical functions. We end this section by emphasizing that the only approximation introduced in the derivation of the equations of motion presented here is the truncation up to second order in the interaction strength. These equations depict the nonlinear and non-Markovian quantum dynamics, which we consider as the primary distinguishing features of this work. It supersedes what the second order kinetic theories currently presented can do, their going beyond the HFB approximation notwithstanding. For example Ref. \[13\] presents a kinetic theory approach that includes binary interactions to second order in the interaction potential but uses the Markovian approximation. In Ref. \[14\] the authors gave a non-Markovian generalization to the quantum kinetic theory derived by Walser et. al. \[15\] by including memory effects. However in that work symmetry breaking fields, $\phi$ and anomalous fluctuations $m$ are neglected.

## 7.2 Conservation Laws

For a closed (isolated) system the mean total number of particles $N$ and energy are conserved quantities as they are the constants of motion for the dynamical equations.

Particle number conservation is a consequence of the invariance of the Hamiltonian under a global phase change. The mean total number of particles is given by
\[ \langle \hat{N} \rangle = \sum_i \langle \hat{\Phi}_i \hat{\Phi}_i \rangle = \sum_i \left( |\phi_i|^2 + \rho^{(F)}_{ii} - \frac{1}{2} \right) \]  

(62)

\[ \langle \hat{N} \rangle = N. \]

The kinetic equation for \( N \) is then

\[ \frac{d}{dt} \langle \hat{N}(t) \rangle = \sum_i 2 \text{Re} \left( \phi_i(t) \frac{\partial}{\partial t} \phi_i^*(t) \right) + \lim_{t' \rightarrow t} \left( \frac{\partial}{\partial t} \rho^{(F)}_{ii}(t,t') + \frac{\partial}{\partial t'} \rho^{(F)}_{ii}(t',t) \right) \]

(63)

(63)

All three approximations we have considered, namely, HFB, \( 1/N \) expansion and full second order expansion, conserve particle number. This can be shown by plugging in the kinetic equation of \( \langle \hat{N}(t) \rangle \) the equation of motion for the mean field and the normal statistical propagator and cancelling terms. It is important to note that even though total population is always conserved there is always a transfer of population between condensate and non-condensate atoms.

While number conservation can be proved explicitly, to prove total energy conservation is not obvious as the Hamiltonian cannot be represented as a linear combination of the relevant operators. It is clear that the exact solution of a closed system is unitary in time and hence disallows any dissipation. However, the introduction of approximation schemes that truncate the infinite hierarchy of correlation functions at some finite order with causal boundary conditions may introduce dissipation \[6\].

To discuss energy conservation we can use the phi-derivable criteria \[37\] which states that nonequilibrium approximations in which the self energy \( \Sigma \) is of the form \( \delta \Phi / \delta G \), with \( \Phi \) a functional of \( G \), conserve particle number, energy and momentum. All the approximations we consider in this paper are phi derivable and thus they obey energy, particle number and momentum conservation laws. For HFB, \( \Phi = \Gamma^{(1)}_2 \), for the full second order expansion, \( \Phi = \Gamma^{(1)}_2 + \Gamma^{(2)}_2 \) and for the second order next to leading order \( 1/N \) expansion, \( \Phi = \Gamma^{(1)}_2 + \Gamma^{(2)}_2/1/N \).

See Eqs. \[24\], \[42\], \[53\] and \[61\]. For a detailed discussion of the complete next to leading order \( 1/N \) expansion see Refs. \[15\], \[16\] and references therein.

### 7.3 Zero mode fluctuations

The spectrum of fluctuations above the condensate includes a zero mode. This mode is the Goldstone boson associated with the breaking of global phase invariance by the condensate. It is analogous to the collective modes which arise in the spectrum of fluctuations around a bubble \[38\]. The zero mode is essentially non-perturbative. In linearized theory, it introduces an artificial infrared divergence in low dimensional models. For this reason linearized theory is actually improved if the contribution from this mode is neglected all together \[39\]. A different way to deal with the zero mode has been proposed by Gardiner \[40\] and Morgan \[21\]. Here the theory is written in terms of operators which exchange particles between zero and nonzero modes, conserving the total particle number, and one further operator which changes total particle number. The contribution from the zero mode is then subtracted by expressing the normal and anomalous densities in terms of the former alone. However, from a physical point of view the zero mode exists and is quantum in nature. We may think of it as the limit of Gardiner and Zoller’s \[41\] "condensate band "when the width of the band shrinks to zero. There are both fundamental and practical reasons why isolating and subtracting the zero mode is not as compelling in our case as in the problems discussed by Gardiner and Morgan. In the problem we discuss, the initial state is a coherent state rather than a proper state of the total particle number. As the total particle number is not very high quantum fluctuations in the total particle number are real, and non-negligible. Discarding these fluctuations would spoil the integrity of the formalism. Also, because the 2PI formalism goes beyond the linearized approximation, the zero mode does not have the impact it has in the linearized formalism and it is
not clear that subtracting it necessarily leads to a better approximation. Therefore, in this paper we shall not attempt to isolate the contributions from the zero mode. A full non-perturbative treatment in the future is certainly desirable.

8 Numerical Implementation

8.1 Exact Solution

The fully quantal solution was found by evolving in time the initial state with the Bose-Hubbard Hamiltonian given by Eq. (1), so that $|\varphi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\varphi(0)\rangle$ with $|\varphi(0)\rangle = e^{-N/2\sqrt{N}\Phi_0}|0\rangle_0\prod_{i\neq 0}|0\rangle_i$. To do the numerical calculations we partitioned the Hilbert space in subspaces with fixed number of atoms and propagated independently the projections of the initial state on the respective subspaces. A subspace with $N_n$ number of atoms and $I$ number of wells is spanned by $(N_n+I-1)!$ states. This procedure could be done because the Hamiltonian commutes with the number operator $\sum_i \Phi_i^\dagger \Phi_i$, and thus during the dynamics the different subspaces never get mixed. The number of subspaces used for the numerical evolution were such that no change in plots of the dynamical observables was detected by adding another subspace. Generally for $N$ atoms in the initial state, this condition was achieved by including the subspaces between $N - 4\sqrt{N}$ and $N + 4\sqrt{N}$ atoms.

8.2 Numerical Algorithm for the approximated solution

The time evolution equations obtained in Sec. 7 are nonlinear integro-differential equations. Though the equations are very complicated, they can be solved on a computer. The important point to note is that all equations are casual in time, and all quantities at some later time $t_f$ can be obtained by integration over the explicitly known functions for times $t \leq t_f$.

For the numerical solution we employed a time discretization $t = na_t$, $t' = ma_t$, and took the advantage that, due to the presence of the lattice the spatial dimension is discrete (indices $i$ and $j$). The discretized equations for the time evolution of the matrices $\rho_{ijnn}^{(F,\rho)}$, $m_{ijnn}^{(F,\rho)}$ and $\phi_{im}$, advance time step wise in the $n$-direction for fixed $m$. Due to the symmetries of the matrices only half of the $(n,m)$ matrices have to be computed and the values $\rho_{ijnn} = -i$, $m_{ijnn} = 0$ are fixed for all time due to the bosonic commutation relations. As initial conditions one specifies $\rho_{ij00}^{(F,\rho)}$, $m_{ij00}^{(F,\rho)}$ and $\phi_{i0}$.

To ensure that the discretized equations retain the conservation properties present in the continuous ones one has to be very careful in the evolution of the diagonal terms of $\rho_{iinn}$ and take the limit $m \to n$ in a proper way:

\begin{align}
(\rho)_{ijn+1n+1}^{(F,\rho)} - \rho_{ijnn}^{(F,\rho)} &= \left(\rho_{ijn+1n}^{(F,\rho)} - \rho_{ijnn}^{(F,\rho)}\right) \pm \left(\rho_{ijnn}^{(F,\rho)} - \rho_{ijnn}^{(F,\rho)}\right), \\
(\rho)_{ijn+1n+1}^{(F,\rho)} - m_{ijnn}^{(F,\rho)} &= \left(m_{ijn+1n}^{(F,\rho)} - m_{ijnn}^{(F,\rho)}\right) \pm \left(m_{ijnn}^{(F,\rho)} - m_{ijnn}^{(F,\rho)}\right),
\end{align}

with the positive sign for the statistical propagators, $(F)'s$, and negative for the spectral ones, $(\rho)'s$. We use the fourth order Runge-Kutta algorithm to propagate the local part of the equations and a regular one step Euler method to iterate the non local parts. For the integrals we use the standard trapezoidal rule. Starting with $n = 1$, for the time step $n + 1$ one computes successively all entries with $m = 0 \ldots \ldots , n, n + 1$ from known functions evaluated at previous times.

The time step $a_t$ was chosen small enough so that convergence was observed, that is, further decreasing it did not change the results. The greater the parameter $UN/J$ the smaller the time step required. The main numerical limitation of the 2PI approximation is set by the time integrals, which make the numerical calculations time and memory consuming. However, within a typical numerical precision it was typically not necessary to keep all the past of the two point functions in the memory. A characteristic time, after which the
influence of the early time in the late time behavior is given by the inverse damping rate. This time is described by the exponential damping of the two-point correlator at time \( t \) with the initial time \( \tau_0 \). In our numerics we extended the length of the employed time interval until the results did not depend on it. In general, it was less than the inverse damping rate. We used for the calculations a single PII 400 MH workstation with 260 Mb of memory. For a typical run 1-2 days of computational time were required.

8.3 Initial conditions and parameters

To model the patterned loading the initial conditions assumed for the numerical solutions were:

\[
\phi_{i0} = N\delta_{i0}, \quad \rho_{ij00}^{(F)} = \frac{1}{2}\delta_{ij}, \quad \rho_{ij00}^{(\rho)} = -i\delta_{ij} \quad \text{and} \quad m_{ij00}^{(F)} = m_{ij00}^{(\rho)} = 0.
\]

They correspond to an initial coherent state with \( N \) atoms in the initial populated well.

To study the kinetic energy dominated regime we chose for the simulations three different sets of parameters:

- The first set was chosen to be in the very weak interacting regime, \( I = 3, N = 6, J = 1 \) and \( U/J = 1/30 \). With this choice we wanted to show the validity of a mean field approach to describe this regime and the corrections introduced by the higher order approximations.
- The second set of parameters were \( I = 3, N = 8, J = 1 \) and \( U/J = 1/3 \). In this regime the kinetic energy is big enough to allow tunneling but the effect of the interactions are crucial in the dynamics. Comparing with the exact solution we could show the break-down of the mean field approximation.

At the mean field level (using the DNLSE) for a given number of wells, the only relevant parameter for describing the dynamics of the system is the ratio \( UN/J \). For a fixed \( UN/J \) the mean field dynamics is independent of the number of atoms in consideration. This is not the case in the exact solution where both \( UN/J \) and \( N \) are important. As \( N \) is increased the bigger the population in the initial coherent matter field and therefore we expect a better agreement of the truncated theories with the exact solution. To study the dependence of the dynamics on the total number of atoms, the third set of parameters in our solutions were chosen to be \( I = 2, J = 1/2 \) and fixed \( NU/J = 4 \) but we changed the number of atoms from 20 to 80. To increase the number of atoms in the calculations we had to reduce the number of wells to two due to the fact that the dimension of the Hilbert space scales very badly with \( N \) and \( I \).

9 Results and Discussions

In Figs. 3 to 7 we show our numerical results. We focus our attention on the evolution of the condensate population per well, \( |\phi_i(t)|^2 \), the total atomic population per well, \( |\phi_i|^2 + \rho_{ii}^{(F)}(t, t) - \frac{1}{2} \), the depletion per well or atoms out of the condensate, \( \rho_{ii}^{(F)}(t, t) - \frac{1}{2} \), and the total condensate population, \( \sum_i |\phi_i(t)|^2 \). The total population is also explicitly shown in the figures to emphasize number conservation.

The quasi-momentum distribution of the atoms released from the lattice is important because it is one of the most easily accessible quantities from an experiment. The quasi-momentum distribution function \( n_k(t) \) is defined as

\[
n_k(t) = \frac{1}{I} \sum_{i,j} e^{ik(i-j)} \left\langle \Phi_i^\dagger(t) \Phi_j(t) \right\rangle, \quad (66)
\]

where the quasi-momentum \( k \) can assume discrete values which are integral multiples of \( \frac{2\pi}{Ia} \), with \( I \) the total number of lattice sites and \( a \) the lattice spacing.

The basic features of the plots can be summarized as follows:

In the very weak interacting regime (Fig. 3) the dynamics of the atomic population per well is almost like Rabi oscillations. Notice that even though there are three wells, periodic boundary conditions enforce equal evolution of the initial empty ones. In this regime damping effects remains very small for the time depicted in the plots. The numerical simulations show a general agreement between the different approaches with the exact solution. The effect of including higher order terms in the equations of motion introduce small corrections.
which improve the agreement with the exact dynamics. This shows up in the plots of the condensate population and depletion, where the small differences can be appreciated better. The second order $1/N$ expansion gives an improvement over the HFB and the complete second order perturbative expansion almost matches perfectly with the exact solution. In the duration depicted in the plots of Fig. 3 the total condensate constitutes an important fraction of the total population. Regarding the quasi-momentum distribution we observe that similar to the spatial distribution where the initial configuration and periodic boundary conditions reduce the three well system to a double well one, they enforce equal evolution of the $\pm \frac{2\pi}{3}$ quasimomentum intensities. The $k = 0$ and $\pm \frac{2\pi}{3}$ intensities oscillate with the same frequency as the atomic population per well, both are also well described by the approximations in consideration.

In the intermediate regime we can see the effect of the interactions in the dynamics. They modulate the oscillations in the population per well and scatter the atoms out of the condensate.

1. In Figs. 4 we plot the numerical solution for the parameters $I = 3, N = 8, J = 1$ and $U/J = 1/3$. Different from the very weak interacting regime only at the very early times all three approximations are close to the exact solution. Even though any of them are good after the first oscillation the HFB approximation is the only one that fails to capture the exponential decrease of the condensate population. This is expected, because even though this approximation goes beyond mean field theory and takes into account the most important scattering effects, it includes the effects of collisions only indirectly through energy shifts, and breaks down outside the collisionless regime where multiple-scattering effects are important. In contrast, the exponential decay of the condensate is present in the second order approximations. Non local parts of the self-energy included in them encode scattering effects responsible for damping. It is important to point out that, even though we observe the collapse of the condensate population, the total population is always conserved: As the condensate population decreases, the number of atoms out of the condensate increases.

2. Comparing the two second order approaches we observe that the full second order expansion gives a better description of the dynamics than the $1/N$ solution only in the regime when the perturbative solutions are close to the exact dynamics. As soon as the third order terms start to be important the large $1/N$ expansion gives a better qualitative description. This behavior is going to be appreciated better in figs. 5 to 7 as the number of atoms is increased (see discussion below).

We observe as a general issue in this regime that, regardless of the fact that the second order solutions capture well the damping effects, as soon as the condensate population decreases to a small percentage of the total population, they depart from the exact dynamics: the second order approaches predict faster damping rates. The over damping is more severe in the dynamics of the population per well than in the condensate dynamics. The failure can be understood under the following lines of reasoning. At zero temperature condensate atoms represent the most "classical" form of a matter wave. When they decay, the role of quantum correlations become more important. At this point the higher order terms neglected in the second order approximations are the ones that lead the dynamical behavior. Thus, to have a more accurate description of the dynamics after the coherent matter field has decayed one needs a better treatment of correlations.

Damping effects are also quite noticeable in the quantum evolution of the quasi-momentum intensities. Similar to what happens to the spatial observables, the HFB approximation fails completely to capture the damping effects present in the evolution of the Fourier intensities whereas the second order approaches overestimate them.

3. In Figs. 5 to 7 we explore the effect of the total number of atoms on the dynamics. In the plots we show the numerical solutions found for a double well system with fix ratio $UN/J = 4$ and three different values of $N$: $N=20,40$ and 80. We present the results obtained for the evolution of the atomic population per well in Fig. 5, the condensate population per well and total condensate population in Fig. 6 and the
quasi-momentum intensities in Fig. 7. To make the comparisons easier we scaled the numerical results obtained for the three different values of \( N \) by dividing them by the total number of atoms. In this way for all the cases we start with an atomic population of magnitude one in the initial populated well.

In the exact dynamics we see that as the number of atoms is increased the damping effects occur at slower rates. This feature can be noticed in the quantum dynamics of all of the observables depicted in the plots 5 to 7. The decrease of the damping rates as the number of atoms is increased is not surprising because by changing the number of atoms we affect the quantum coherence properties of the system. As shown in Ref. [20], the collapse time of the condensate population is approximately given by

\[
t_{\text{coll}} \sim \frac{t_{\text{rev}}}{\sigma}
\]

where \( \sigma \) is the variance of the initial atomic distribution and \( t_{\text{rev}} \) is the revival time which depends on the detailed spectrum for the Hamiltonian. In the kinetic energy dominated regime \( t_{\text{rev}} \approx \hbar N/J \) (see Ref. [19]), thus

\[
t_{\text{coll}} \sim \frac{\hbar}{\sigma J}.
\]

For our initial conditions the variance is proportional to

\[
\sigma = \sqrt{N}
\]

so

\[
t_{\text{coll}} \sim \sqrt{N}.
\]

Besides damping rates, the qualitative behavior of the exact quantum dynamics is not affected very much as the number of atoms is increased for a fixed \( UN/J \).

The improvement of the 2PI approximations as \( N \) is increased, as a result of the increase in the initial number of coherent atoms is in fact observed in the plots. Even though the problem of underdamping in the HFB approximation and the overdamping in the second order approaches are not cured, as the number of atoms is increased, we do observe a better matching with the full quantal solution. The \( 1/N \) expansion shows the fastest convergence. Perhaps this issue can be more easily observed in the quasi-momentum distribution plots, Fig. 7. The better agreement of the \( 1/N \) expansion relies on the fact that even though the number of fields is only two in our calculations the \( 1/N \) expansion is an expansion about a strong quasiclassical field configuration.

10 Conclusions

In this work we have used the CTP functional formalism for 2PI Green’s functions to describe the nonequilibrium dynamics of a condensate loaded in an optical lattice on every third lattice sites. We have carried out the analysis up to second order in the interaction strength. This approximation is introduced so as to make the numerical solution manageable, but it is sufficient to account for dissipative effects due to multiparticle scattering that are crucial even at early times. Our formulation is capable of capturing the salient features of the system dynamics in the regime under consideration, such as the decay of the condensate population and the damping of the oscillations of the quasi-momentum and population per well unaccounted for in the HFB approximation. However, at the point where an important fraction of the condensate population has been scattered out, the second order approximations used here predict an overdamped dynamics. To improve on this, a better treatment of higher correlations is required. One might try to include the full next to leading order large \( N \) expansion without the truncation to second order as done in Ref. [16] but it is not obvious that this will lead to the required improvement. Alternatively, one may try to adopt a stochastic approach, but the challenge will be shifted to the derivation of a noise term (which is likely to be both colored and multiplicative) which contains the effects of these higher correlations and the solution of the stochastic equations. We hope to address this aspect of the problem in a future work.

Even though, as is clear in this paper, the second order 2PI approximations fail to capture the fully correlated dynamics in the system, it has been proved to work at intermediate times when correlations are not negligible and standard mean field techniques fail poorly. Because of its success in describing moderately correlated regimes, the second order approximations could become a useful tool for describing experimental situations as the collapsing or colliding condensates experiments where striking dynamical behavior such as collisional loss of condensate atoms has been observed.

In summary, we have presented a new approach for the description of the nonequilibrium dynamics of a Bose-Einstein condensate and fluctuations in a closed quantum field system. The formalism allows one to go beyond the well known HFB approximation and to incorporate the nonlinear and non-Markovian aspects of
the quantum dynamics as manifest in the dissipation and fluctuations phenomena. The 2PI effective action formalism provides a useful framework where the mean field and the correlation functions are treated on the same footing self-consistently and that respects conservations of particle number and energy. The CTP formalism ensures that the dynamical equations of motion are also causal. In their current form scattering terms non local in time are hard to estimate analytically and numerically demanding. However, this systematic approach can be used as a quantitative means to obtain solutions in different regimes and make comparisons with kinetic theory results where a Markovian approximation is assumed.

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**Appendix 1: Mode Expansion of the HFB Equations**

To decouple the HFB equations we apply the well known Bogoliubov transformation to the fluctuation field:

$$\varphi_j(t) = \sum_q u^q_i(t) \hat{\alpha}_q - v^q_i(t) \hat{\alpha}^\dagger_q, \quad (A-1)$$

where $(\hat{\alpha}_q, \hat{\alpha}^\dagger_q)$ are time independent creation and annihilation quasiparticle operators and all the time dependence is absorbed in the amplitudes $\{u^q_i(t), v^q_i(t)\}$. To ensure that the quasi-particle transformation is canonical, the amplitudes $\{u^q_i(t), v^q_i(t)\}$ have to fulfill the following relations:

$$\sum_i u^q_i(t) u^*_{i\ell}(t) - u^q_i(t) v^*_{i\ell}(t) = \delta_{q\ell}, \quad (A-2)$$

$$\sum_i u^q_i(t) v^*_{i\ell}(t) - u^q_i(t) u^*_{i\ell}(t) = 0. \quad (A-3)$$

In the zero temperature limit, where $\langle \hat{\alpha}^\dagger_q \hat{\alpha}_k \rangle = 0$, the statistical and spectral functions take the form

$$\rho^{(F)}_{ij}(t,t') = \frac{1}{2} \sum_q \left( u^q_i(t) v^*_{j\ell}(t') + u^q_j(t') v^*_{i\ell}(t) \right), \quad (A-4)$$

$$\rho^{(o)}_{ij}(t,t') = i \sum_q \left( u^q_i(t) v^*_{j\ell}(t') - u^q_j(t') v^*_{i\ell}(t) \right), \quad (A-5)$$

$$m^{(F)}_{ij}(t,t') = \frac{1}{2} \sum_q \left( u^q_i(t) v^*_{j\ell}(t') + u^q_j(t') v^*_{i\ell}(t) \right), \quad (A-6)$$

$$m^{(o)}_{ij}(t,t') = i \sum_q \left( u^q_i(t) v^*_{j\ell}(t') - u^q_j(t') v^*_{i\ell}(t) \right). \quad (A-7)$$

$^3$The HFB approximation can be seen as a quadratic approximation of the Hamiltonian in which third and quartic terms are reduced to linear and quadratic forms by factorizing them in a self-consistent Gaussian approximation. Any quadratic Hamiltonian can be diagonalized exactly and this is achieved by transforming to a quasi-particle basis, $\{\hat{\alpha}_q\}$. The requirement of the transformation to be canonical means that it preserves commutation relation and leads to bosonic quasi-particles.
Replacing Eqs. (A-4) - (A-7) into Eqs. (A-8) - (A-10) and using the constraints (A-2)-(A-3) we recover the standard time dependent equations for the quasiparticle amplitudes [23]:

\[ i\hbar \partial_t \phi_i(t) = -J(\phi_{i+1}(t) + \phi_{i-1}(t)) + U(|\phi_i(t)|^2 + 2\rho^{(F)}_{ii}(t,t))\phi_i(t) + Um_{ii}^{(F)}(t,t)\phi_i^*(t), \]  
\[ (A-8) \]

\[ i\hbar \partial_t u^q_i(t) = -J(u^q_{i+1}(t) + u^q_{i-1}(t)) + 2U(|\phi_i(t)|^2 + \rho^{(F)}_{ii}(t,t))u^q_i(t) - U(m_{ii}^{(F)}(t,t) + \phi_i(t)^2)u^q_i(t), \]  
\[ (A-9) \]

\[ -i\hbar \partial_t v^q_i(t) = -J(v^q_{i+1}(t) + v^q_{i-1}(t))) + 2U(|\phi_i(t)|^2 + \rho^{(F)}_{ii}(t,t))v^q_i(t) - U(m_{ii}^{(F)}(t,t) + \phi_i(t)^2)v^q_i(t), \]  
\[ (A-10) \]

Equations (A-8) - (A-10) correspond to a set of \( I(2I + 1) \) coupled ordinary differential equations, where \( I \) is the total number of lattice sites. They can be solved using standard time propagation algorithms. Once the time dependent quasiparticle amplitudes is calculated we can derive the dynamics of physical observables constructed from them as a function of time, such as the average number of particles in a well \( n_i(t) \), etc.

**Appendix 2: Second order equations of Motion**

Hereunder we explicitly write the equations of motion of the \( 1/N \) and full second order approximations.

To simplify the notation let us introduce the functions

\[ \Omega_{ij}^{(F)} [f, g] = f_{ij}^{(F)}(t_i, t_j)g_{ij}^{(F)}(t_i, t_j) - \frac{1}{4} \left( f_{ij}^{(\rho)}(t_i, t_j)g_{ij}^{(\rho)}(t_i, t_j) - f_{ij}^{(\rho)}(t_i, t_j)g_{ij}^{(\rho)}(t_i, t_j) \right), \]  
\[ (B-1) \]

\[ \Omega_{ij}^{(\rho)} [f, g] = f_{ij}^{(F)}(t_i, t_j)g_{ij}^{(\rho)}(t_i, t_j) + f_{ij}^{(\rho)}(t_i, t_j)g_{ij}^{(F)}(t_i, t_j). \]  
\[ (B-2) \]

Using the spectral and statistical functions and setting \( N \) equal to 2 the equations of motion derived in Sec. 7 can be written as:

1. Full second order expansion
   
   If we take the complete contribution of the *setting-sun* and *basket-ball* diagrams the equations of motion take the form

\[ i\hbar \partial_t \phi_i = -J(\phi_{i+1}(t_i) + \phi_{i-1}(t_i)) + U(|\phi_i|^2 + 2\rho^{(F)}_{ii})\phi_i + Um_{ii}^{(F)}\phi_i^* \]  
\[ (B-3) \]

\[ -2U^2 \sum_k \int_{t_0}^{t_i} dt_k \left( \phi_k \Omega_{ik}^{(\rho)} [\rho, \rho^*] + \phi_k \Omega_{ik}^{(\rho)} [m, m^*] + \phi_k \Omega_{ik}^{(\rho)} [m, \rho] \right) \rho_k^{(F)}, \]

\[ +2U^2 \sum_k \int_{t_0}^{t_i} dt_k \left( \phi_k \Omega_{ik}^{(\rho)} [\rho, \rho^*] + \phi_k \Omega_{ik}^{(\rho)} [m, m^*] + \phi_k \Omega_{ik}^{(\rho)} [m, \rho] \right) \rho_k^{(F)} \]

\[ +2U^2 \sum_k \int_{t_0}^{t_i} dt_k \left( \phi_k \Omega_{ik}^{(\rho)} [\rho, \rho^*] + \phi_k \Omega_{ik}^{(\rho)} [m, m^*] + \phi_k \Omega_{ik}^{(\rho)} [m, \rho] \right) m_k^{(\rho)}, \]
\(-i\hbar \partial_t \rho_{ij}^{(F)} = -J(\rho_{i+1j}^{(F)}(t_i, t_j) + \rho_{i-1j}^{(F)}(t_i, t_j)) + 2U(|\phi_i|^2 + \rho_{ii}^{(F)})\rho_{ij}^{(F)} + U(m_{ii}^{(F)} + \phi_i^2)m_{ij}^{(F)} \) (B-4)

\[-2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( \phi_i \phi_k^* \Omega_{ik}^{(F)}[\rho, \rho] + 2\phi_i \phi_k \Omega_{ik}^{(F)}[\rho, m^*] + 2\phi_i^* \phi_k^* \Omega_{ik}^{(F)}[m, \rho] \right) \rho_{kj}^{(F)} \]

\[-2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( \Omega_{ik}^{(F)}[\rho, \Delta] + 2\phi_i^* \phi_k \left( \Omega_{ik}^{(F)}[\rho, \rho^*] + \Omega_{ik}^{(F)}[m, m^*] \right) \right) \rho_{kj}^{(F)} \]

\[-2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( 2\phi_i \phi_k^* \Omega_{ik}^{(F)}[m^*, \rho] + \phi_i \phi_k \Omega_{ik}^{(F)}[m^*, m^*] + 2\phi_i^* \phi_k^* \Omega_{ik}^{(F)}[m, \rho] \right) m_{kj}^{(F)} \]

\[+2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( \Omega_{ik}^{(F)}[\rho, \Delta] + 2\phi_i^* \phi_k \left( \Omega_{ik}^{(F)}[\rho, \rho^*] + \Omega_{ik}^{(F)}[m, m^*] \right) \right) \rho_{kj}^{(F)} \]

\[+2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( 2\phi_i \phi_k^* \Omega_{ik}^{(F)}[m^*, \rho] + \phi_i \phi_k \Omega_{ik}^{(F)}[m^*, m^*] + 2\phi_i^* \phi_k^* \Omega_{ik}^{(F)}[m, \rho] \right) m_{kj}^{(F)} \]

\[-i\hbar \partial_t \rho_{ij}^{(r)} = -J(\rho_{i+1j}^{(r)}(t_i, t_j) + \rho_{i-1j}^{(r)}(t_i, t_j)) + 2U(|\phi_i|^2 + \rho_{ii}^{(r)})\rho_{ij}^{(r)} + U(m_{ii}^{(r)} + \phi_i^2)m_{ij}^{(r)} \) (B-5)

\[-2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( \phi_i \phi_k^* \Omega_{ik}^{(r)}[\rho, \rho] + 2\phi_i \phi_k \Omega_{ik}^{(r)}[\rho, m^*] + 2\phi_i^* \phi_k^* \Omega_{ik}^{(r)}[m, \rho] \right) \rho_{kj}^{(r)} \]

\[-2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( \Omega_{ik}^{(r)}[\rho, \Delta] + 2\phi_i^* \phi_k \left( \Omega_{ik}^{(r)}[\rho, \rho^*] + \Omega_{ik}^{(r)}[m, m^*] \right) \right) \rho_{kj}^{(r)} \]

\[-2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( 2\phi_i \phi_k^* \Omega_{ik}^{(r)}[m^*, \rho] + \phi_i \phi_k \Omega_{ik}^{(r)}[m^*, m^*] + 2\phi_i^* \phi_k^* \Omega_{ik}^{(r)}[m, \rho] \right) m_{kj}^{(r)} \]

\[+2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( \Omega_{ik}^{(r)}[\rho, \Delta] + 2\phi_i^* \phi_k \left( \Omega_{ik}^{(r)}[\rho, \rho^*] + \Omega_{ik}^{(r)}[m, m^*] \right) \right) \rho_{kj}^{(r)} \]

\[+2U^2 \sum_k \int_{t_i}^{t_j} dt_k \left( 2\phi_i \phi_k^* \Omega_{ik}^{(r)}[m^*, \rho] + \phi_i \phi_k \Omega_{ik}^{(r)}[m^*, m^*] + 2\phi_i^* \phi_k^* \Omega_{ik}^{(r)}[m, \rho] \right) m_{kj}^{(r)} \]
\[
\begin{align*}
\text{i}h\partial_t m_{ij}^{(F)} &= -J(m_{i+1,j}^{(F)}(t, t_j) + m_{i-1,j}^{(F)}(t, t_j)) + 2U(|\phi_i|^2 + \rho_{ii}^{(F)})m_{ij}^{(F)} + U(m_{ii}^{(F)} + \phi_i^2)\rho_{ij}^{(F)} \quad (B-6) \\
-2U^2 \sum_k \int_0^{t_i} dt_k \left( 2\phi_i^* \rho_{kk}^{(F)} [m, \rho^*] + \phi_i^* \rho_{kk}^{(F)} [m, m] + 2\phi_i \rho_{kk}^{(F)} [\rho, m] \right) \rho_{kj}^{(F)} \\
-2U^2 \sum_k \int_0^{t_i} dt_k \left( \Omega_{ik}^{(F)} [m, \gamma] + 2\phi_i \rho_{kk}^{(F)} \left( \Omega_{ik}^{(F)} [\rho, \rho^*] + \Omega_{ik}^{(F)} [m, m^*] \right) \right) \rho_{kj}^{(F)} \\
-2U^2 \sum_k \int_0^{t_i} dt_k \left( \phi_i^* \rho_{kk}^{(F)} [\rho^*, \rho^*] + \phi_i^* \rho_{kk}^{(F)} [\rho^*, m] + 2\phi_i \rho_{kk}^{(F)} [m^*, \rho^*] \right) m_{kj}^{(F)} \\
-2U^2 \sum_k \int_0^{t_i} dt_k \left( \Omega_{ik}^{(F)} [\rho^*, \Delta] + 2\phi_i \rho_{kk}^{(F)} \left( \Omega_{ik}^{(F)} [\rho, m^*] + \Omega_{ik}^{(F)} [m, m^*] \right) \right) m_{kj}^{(F)} \\
+2U^2 \sum_k \int_0^{t_i} dt_k \left( 2\phi_i^* \rho_{kk}^{(F)} [m, \rho^*] + \phi_i^* \rho_{kk}^{(F)} [m, m] + 2\phi_i \rho_{kk}^{(F)} [\rho, m^*] \right) \rho_{kj}^{(F)} \\
+2U^2 \sum_k \int_0^{t_i} dt_k \left( \Omega_{ik}^{(F)} [m, \gamma] + 2\phi_i \rho_{kk}^{(F)} \left( \Omega_{ik}^{(F)} [\rho, \rho^*] + \Omega_{ik}^{(F)} [m, m^*] \right) \right) \rho_{kj}^{(F)} \\
+2U^2 \sum_k \int_0^{t_i} dt_k \left( \phi_i^* \rho_{kk}^{(F)} [\rho^*, \rho^*] + \phi_i^* \rho_{kk}^{(F)} [\rho^*, m] + 2\phi_i \rho_{kk}^{(F)} [m^*, \rho^*] \right) m_{kj}^{(F)} \\
+2U^2 \sum_k \int_0^{t_i} dt_k \left( \Omega_{ik}^{(F)} [\rho^*, \Delta] + 2\phi_i \rho_{kk}^{(F)} \left( \Omega_{ik}^{(F)} [\rho, m^*] + \Omega_{ik}^{(F)} [m, m^*] \right) \right) m_{kj}^{(F)},
\end{align*}
\]

\[
\begin{align*}
\text{i}h\partial_t m_{ij}^{(\rho)} &= -J(m_{i+1,j}^{(\rho)}(t, t_j) + m_{i-1,j}^{(\rho)}(t, t_j)) + 2U(|\phi_i|^2 + \rho_{ii}^{(\rho)})m_{ij}^{(\rho)} + U(m_{ii}^{(\rho)} + \phi_i^2)\rho_{ij}^{(\rho)} \quad (B-7) \\
+2U^2 \sum_k \int_{t_j}^{t_i} dt_k \left( 2\phi_i^* \rho_{kk}^{(\rho)} [m, \rho^*] + \phi_i^* \rho_{kk}^{(\rho)} [m, m] + 2\phi_i \rho_{kk}^{(\rho)} [\rho, m] \right) \rho_{kj}^{(\rho)} \\
+2U^2 \sum_k \int_{t_j}^{t_i} dt_k \left( \Omega_{ik}^{(\rho)} [m, \gamma] + 2\phi_i \rho_{kk}^{(\rho)} \left( \Omega_{ik}^{(\rho)} [\rho, \rho^*] + \Omega_{ik}^{(\rho)} [m, m^*] \right) \right) \rho_{kj}^{(\rho)} \\
+2U^2 \sum_k \int_{t_j}^{t_i} dt_k \left( \phi_i^* \rho_{kk}^{(\rho)} [\rho^*, \rho^*] + \phi_i^* \rho_{kk}^{(\rho)} [\rho^*, m] + 2\phi_i \rho_{kk}^{(\rho)} [m^*, \rho^*] \right) m_{kj}^{(\rho)} \\
+2U^2 \sum_k \int_{t_j}^{t_i} dt_k \left( \Omega_{ik}^{(\rho)} [\rho^*, \Delta] + 2\phi_i \rho_{kk}^{(\rho)} \left( \Omega_{ik}^{(\rho)} [\rho, m^*] + \Omega_{ik}^{(\rho)} [m, m^*] \right) \right) m_{kj}^{(\rho)},
\end{align*}
\]

with

\[
\begin{align*}
\Delta_{ij}^{(F,\rho)} &= \Omega_{ij}^{(F,\rho)} [\rho, \rho^*] + 2\Omega_{ij}^{(F,\rho)} [m, m^*], \\
\gamma_{ij}^{(F,\rho)} &= 2\Omega_{ij}^{(F,\rho)} [\rho, \rho^*] + \Omega_{ij}^{(F,\rho)} [m, m^*].
\end{align*}
\]
\[ i\hbar \partial_t \phi_i = -J(\phi_{i+1}(t_i) + \phi_{i-1}(t_i)) + U(|\phi_i|^2 + 2\rho^{(F)}_{ii} \phi_i + U m^{(F)}_{ii} \phi_i^* ) \quad (B-10) \]

\[ -U^2 \sum_k \int_0^{t_1} dt_k \Pi^{(F)}_{ik}(\phi_k \rho^{(F)}_{kk} + \phi_k^* m^{(F)}_{kk}) + U^2 \sum_k \int_0^{t_1} dt_k \Pi^{(F)}_{ik}(\phi_k \rho^{(F)}_{kk} + \phi_k^* m^{(F)}_{kk}) , \]

\[ -i\hbar \partial_t \rho^{(F)}_{ij} = -J(\rho^{(F)}_{i+1,j}(t_i, t_j) + \rho^{(F)}_{i-1,j}(t_i, t_j)) + 2U(|\phi_i|^2 + \rho^{(F)}_{ii}) \rho^{(F)}_{ij} + U (m^{(F)}_{ii} + \phi_i^2) m^{(F)}_{ij} \quad (B-11) \]

\[ -U^2 \sum_k \int_0^{t_1} dt_k \left( \phi_i \phi_k^* \Omega^{(F)}_{ik} [\rho, \rho] + \phi_i \phi_k \Omega^{(F)}_{ik} [\rho, m^*] + \phi_i^* \phi_k^* \Omega^{(F)}_{ik} [m, \rho] \right) \rho^{(F)}_{kj} \]

\[ -U^2 \sum_k \int_0^{t_1} dt_k \left( \Omega^{(F)}_{ik} [m, \Pi] + \phi_i^* \phi_k \left( 2\Omega^{(F)}_{ik} [\rho, \rho^*] + \Omega^{(F)}_{ik} [m, m^*] \right) \right) m^{(F)}_{kj} \]

\[ -U^2 \sum_k \int_0^{t_1} dt_k \left( \Omega^{(F)}_{ik} [m, \Pi] + \phi_i^* \phi_k \left( 2\Omega^{(F)}_{ik} [\rho, \rho^*] + \Omega^{(F)}_{ik} [m, m^*] \right) \right) m^{(F)}_{kj} \]

\[ +U^2 \sum_k \int_0^{t_1} dt_k \left( \phi_i \phi_k^* \Omega^{(F)}_{ik} [\rho, \rho] + \phi_i \phi_k \Omega^{(F)}_{ik} [\rho, m^*] + \phi_i^* \phi_k^* \Omega^{(F)}_{ik} [m, \rho] \right) \rho^{(F)}_{kj} \]

\[ +U^2 \sum_k \int_0^{t_1} dt_k \left( \Omega^{(F)}_{ik} [\rho, \Pi] + \phi_i^* \phi_k \left( 2\Omega^{(F)}_{ik} [\rho, \rho^*] + \Omega^{(F)}_{ik} [m, m^*] \right) \right) m^{(F)}_{kj} \]

\[ +U^2 \sum_k \int_0^{t_1} dt_k \left( \phi_i \phi_k^* \Omega^{(F)}_{ik} [\rho, \rho] + \phi_i \phi_k \Omega^{(F)}_{ik} [\rho, m^*] + \phi_i^* \phi_k^* \Omega^{(F)}_{ik} [m, \rho] \right) \rho^{(F)}_{kj} \]

\[ +U^2 \sum_k \int_0^{t_1} dt_k \left( \Omega^{(F)}_{ik} [m, \Pi] + \phi_i^* \phi_k \left( 2\Omega^{(F)}_{ik} [\rho, \rho^*] + \Omega^{(F)}_{ik} [m, m^*] \right) \right) m^{(F)}_{kj} , \]

\[ -i\hbar \partial_t \rho^{(F)}_{ij} = -J(\rho^{(F)}_{i+1,j}(t_i, t_j) + \rho^{(F)}_{i-1,j}(t_i, t_j)) + 2U(|\phi_i|^2 + \rho^{(F)}_{ii}) \rho^{(F)}_{ij} + U (m^{(F)}_{ii} + \phi_i^2) m^{(F)}_{ij} \quad (B-12) \]

\[ -U^2 \sum_k \int_0^{t_1} dt_k \left( \phi_i \phi_k^* \Omega^{(F)}_{ik} [\rho, \rho] + \phi_i \phi_k \Omega^{(F)}_{ik} [\rho, m^*] + \phi_i^* \phi_k^* \Omega^{(F)}_{ik} [m, \rho] \right) \rho^{(F)}_{kj} \]

\[ -U^2 \sum_k \int_0^{t_1} dt_k \left( \Omega^{(F)}_{ik} [\rho, \Pi] + \phi_i^* \phi_k \left( 2\Omega^{(F)}_{ik} [\rho, \rho^*] + \Omega^{(F)}_{ik} [m, m^*] \right) \right) m^{(F)}_{kj} \]

\[ -U^2 \sum_k \int_0^{t_1} dt_k \left( \phi_i \phi_k^* \Omega^{(F)}_{ik} [\rho, \rho] + \phi_i \phi_k \Omega^{(F)}_{ik} [\rho, m^*] + \phi_i^* \phi_k^* \Omega^{(F)}_{ik} [m, \rho] \right) \rho^{(F)}_{kj} \]

\[ +U^2 \sum_k \int_0^{t_1} dt_k \left( \Omega^{(F)}_{ik} [\rho, \Pi] + \phi_i^* \phi_k \left( 2\Omega^{(F)}_{ik} [\rho, \rho^*] + \Omega^{(F)}_{ik} [m, m^*] \right) \right) m^{(F)}_{kj} . \]
\[ i\hbar \partial_t m_{ij}^{(F)} = -J(m_{i+1,j}^{(F)}(t_i, t_j) + m_{i-1,j}^{(F)}(t_i, t_j)) + 2U(|\phi|_i|^2 + \rho_{ij}^{(F)})m_{ij}^{(F)} + U(m^{(F)}_{ii} + \phi_i^2)\rho_{ij}^{(F)} \]  
(B-13)

\[ -U^2 \sum_k \int_{t_i}^{t_f} dt_k \left( \phi_i^* \phi_k \Omega_{ik}^{(p)} [m, \rho^*] + \phi_i^* \phi_k^* \Omega_{ik}^{(p)} [\rho, m] + \phi_i^* \phi_k \Omega_{ik}^{(p)} [\rho, m] \right) \rho_{kj}^{(F)} \]

\[ -U^2 \sum_k \int_{t_i}^{t_f} dt_k \left( \Omega_{ik}^{(p)} [m, \Pi] + \phi_i \phi_k \left( \Omega_{ik}^{(p)} [\rho, \rho^*] + 2\Omega_{ik}^{(p)} [m, m^*] \right) \right) \rho_{kj}^{(F)} \]

\[ -U^2 \sum_k \int_{t_i}^{t_f} dt_k \left( \phi_i^* \phi_k \Omega_{ik}^{(p)} [\rho^*, \rho^*] + \phi_i^* \phi_k^* \Omega_{ik}^{(p)} [\rho, m] + \phi_i^* \phi_k \Omega_{ik}^{(p)} [m, \rho^*] \right) m_{kj}^{(F)} \]

\[ +U^2 \sum_k \int_{t_i}^{t_f} dt_k \left( \phi_i^* \phi_k \Omega_{ik}^{(p)} [m, \rho^*] + \phi_i^* \phi_k^* \Omega_{ik}^{(p)} [\rho, m] + \phi_i^* \phi_k \Omega_{ik}^{(p)} [\rho, m] \right) \rho_{kj}^{(p)} \]

\[ +U^2 \sum_k \int_{t_i}^{t_f} dt_k \left( \Omega_{ik}^{(p)} [\rho, \Pi] + \phi_i \phi_k \left( 2\Omega_{ik}^{(p)} [\rho, \rho^*] + \Omega_{ik}^{(p)} [m, m^*] \right) \right) m_{kj}^{(p)} \]

\[ +U^2 \sum_k \int_{t_i}^{t_f} dt_k \left( \Omega_{ik}^{(p)} [\rho^*, \Pi] + \phi_i \phi_k \left( 2\Omega_{ik}^{(p)} [\rho^*, \rho^*] + \Omega_{ik}^{(p)} [m^*, m^*] \right) \right) m_{kj}^{(p)}, \]

with

\[ \Pi_{ij}^{(F, p)} = \Omega_{ij}^{(F, p)} [\rho, \rho^*] + \Omega_{ij}^{(F, p)} [m, m^*]. \]  
(B-15)

In the above equations we have simplified the notation replacing \( \phi_k(t_k) \) by \( \phi_k \) and \( m_{kj}(t_k, t_j) \) by \( m_{kj} \).

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Figure 1: Comparisons between the exact and the DNLSE solutions for six atoms and three wells. The time is given in units of $\hbar/J$. Top panel, strongly correlated regime ($\gamma = 12$); Middle panel, intermediate regime ($\gamma = 2$) and bottom panel weak interacting regime ($\gamma = 0.2$). The solid line is the DNLSE prediction for the population per well: $|\phi_0(t)|^2$ and $|\phi_{1,2}(t)|^2$ (see Eq. 2), the triangles are used to represent the exact solution for the population per well calculate using the Bose Hubbard Hamiltonian (Eq. 1): $\langle \hat{\Phi}_0^\dagger \hat{\Phi}_0 \rangle$, $\langle \hat{\Phi}_{1,2}^\dagger \hat{\Phi}_{1,2} \rangle$. The pentagons show the condensate population per well calculated from the exact solution: $|\langle \hat{\Phi}_0 \rangle|^2$ and $|\langle \hat{\Phi}_{1,2} \rangle|^2$. Due to the symmetry of the initial periodic conditions the curves for the $i = 1$ and 2 wells are the same in all depicted curves.
Figure 2: Two-loop (upper row) and three-loop diagrams (lower row) contributing to the effective action. Explicitly, the diagram a is what we call the *double-bubble*, b the *setting-sun* and c the *basket-ball*. 
Figure 3: Comparisons between the exact solution (solid line), the HFB approximation (boxes), the second order large $N$ approximation (pentagons) and the full 2PI second order approximation (crosses) for the very weak interacting regime. The parameters used were $I = 3, N = 6, J = 1$ and $U/J = 1/30$. The time is given in units of $\hbar/J$. In the plots where the population, condensate and depletion per well are depicted the top curves correspond to the initially populated well solutions and the lower to the initially empty wells. Notice the different scale used in the depletion plot. In the momentum distribution plot the upper curve correspond to the $k = \pm 2\pi/3$ intensities and the lower one to the $k = 0$ quasi-momentum intensity.
Figure 4: Comparisons for the case $I = 3, N = 8, J = 1$ and $U/J = 1/3$. The time is given in units of $\hbar/J$. In the plots the abbreviation 1st is used for the initially occupied well and 2nd for the initially empty wells. In the quasi-momentum plots $q = 2\pi/a$ is the reciprocal lattice vector with $a$ the lattice spacing.
Figure 5: Comparison between the evolution of the atomic population per well for $I = 2, J = 1/2, NU/J = 4$ and $N = 20, 40$ and $80$. Time is in units of $\hbar/J$. In the plots P1 states for the atomic population in the initially populated wells and P2 for the population in the initially empty wells. The number of atoms $N$ is explicitly shown in each panel. To make easier the comparisons all the plots are scaled by $N$ such that the number of atoms is always normalized to one.
Figure 6: Time evolution of the condensate population per well and the total condensate population. Same parameters than Fig. 5. Time is in units of $\hbar/J$. In the plots C1 states for the condensate population in the initially populated well, C2 for the condensate in the initially empty one and CT for the total condensate population. All the plots are scaled to have the total number of atoms set to one for all the different N cases.
Figure 7: Dynamical evolution of the quasi-momentum intensities. The parameters used were $I = 2$, $J = 1/2$, $NU/J = 4$ and $N = 20, 40$ and $80$. Time is in units of $\hbar/J$. In the plots ko denotes the $k = 0$ quasi-momentum component and k1 the $k = \pi/a$ one ($a$ the lattice spacing). The plots are scaled to set the total quasi-momentum intensity to one for all the different N cases.