Gauge-invariant Effective Action for the Dynamics of Bose-Einstein condensates with a fixed number of atoms

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In this paper we present a particle-number-conserving (PNC) functional formalism to describe the dynamics of a cold bosonic gas. Treating the total number of particles as a constraint, whereby the phase invariance of the theory becomes local in time, we study this U(1) gauge theory using DeWitt’s ”gauge invariant effective action” techniques. Our functional formulation and earlier PNC proposals are shown to yield equivalent results to next-to-leading order in an expansion in the inverse powers of the total number of particles. In this more general framework we also show that earlier PNC proposals can be seen as different gauge (and gauge fixing condition) choices within the same physical theory.

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I. INTRODUCTION

Experimental successes in the making of Bose-Einstein condensates (BEC) ushered in a new epoch in atomic and optical physics where precision control of many-atom systems becomes possible. From this we see the rapid development of new tools and techniques where one can construct such systems designed for probing deeper physical issues as well as for more practical purposes (such as quantum information processing QIP). With these advances more sophisticated theoretical methods need be introduced to describe the quantum field and nonequilibrium properties of such systems, addressing the issues related to quantum coherence, correlations, fluctuations and noise. The demand here is to treat the dynamics of strongly correlated quantum systems often in the non-Markovian regimes while respecting the full quantum coherence of the system, meeting the constraints from the set-up and incorporating the effect of noise and fluctuations.

Technically speaking, because any consistent description of quantum fluctuations around a BEC \cite{1} is gapless \cite{2,3}, individual Feynman graphs contributing to quantities of interest may be large. An accurate description of the full quantum dynamics requires resummation of whole classes of graphs. A familiar example is the hard thermal loop techniques developed to describe hot quark-gluon plasmas \cite{4}. These non-perturbative approaches are most easily implemented at the level of the so-called closed time-path effective action (CTPEA)\cite{5,6,7}, closely related to the Feynman - Vernon influence functional for quantum open systems \cite{8}.

The CTPEA allows for two complementary lines of development. If the focus of interest is the evolution of quantum fluctuations and their correlations, then the CTPEA is best combined with the so-called 2 particle irreducible (or Cornwall - Jackiw - Tomboulis) \cite{9} effective action to yield dynamical equations of motion for the correlations themselves \cite{10}. This is in fact the method of choice for dealing with quantum fields in far from equilibrium situations \cite{11}. We should stress that the formulation of the BEC dynamics as a hierarchy of correlations is well known \cite{12}; what sets the EA approach apart is its efficiency with respect to the implementation of nonperturbative resummation of diagrams \cite{13,14,15}.

If the focus of interest is the condensate itself, then the CTPEA may be used to derive a stochastic Gross - Pitaevsky (GP) equation, whereby quantum expectation values of the full theory may be retrieved as averages over the noise. In gravitation and cosmology, a similar problem has led to the derivation of the so-called Einstein-Langevin equation as the centerpiece of the stochastic semiclassical gravity program \cite{16}. Different approaches have been proposed \cite{17} to tackle the interaction of BEC with noncondensate atoms. While these approaches can be shown to be equivalent in the appropriate limits, derivation from the CTPEA enables one to keep track of the non-Markovian nature of dissipation and (colored) noise in a self-consistent manner. This formulation may also be applied to the treatment of decoherence of BEC in microtraps \cite{18}, a
problem similar to environment-induced decoherence in the context of structure formation via the influence functional and CTP techniques [13, 20].

Functional methods have been introduced for the description of BEC dynamics (see, e.g., the lectures of Stoof [6]). The advantages of a field theory approach to many-body systems are well-known: economy in the formulation, flexibility in the use of self-consistency to improve on perturbation theory and the explicit enforcement of conservation laws. There is a vast literature on this subject based on the so-called “symmetry breaking” approach: the theory has a global U(1) symmetry whose breakdown signals condensation. In this approach particle number is conserved but not fixed: there are quantum fluctuations in both the number of particles in the condensate and the total number of particles in the system, only the mean numbers are fixed.

Though convenient this approach contradicts with the actual experimental situation, where the total number of particles is fixed or, if there is loss of atoms, this needs be accounted for in real physical terms. Moreover, in typical experiments the total number of particles (several thousands) is not large enough to make the difference negligible. With precision experimentation, especially for QIP purposes, one should seek a more accurate method. This is the primary motivation for the present work.

To the best of our knowledge, the first proposal for handling a BEC with a fixed number of particles has been put forward by Arnowitt and Girardeau [21], leading to the development of the so-called particle number conserving (PNC) method [22, 23, 24, 25, 26, 27]. The goal of this paper is to formulate a functional PNC approach, and to show the equivalence of the functional and those earlier proposals to next to leading order (NLO) in an expansion in inverse powers of the total number of particles. Let us first see what the problem entails with some technical help.

**A. Field theory approach to BECs**

In recent years, field theory techniques have been systematically applied to the dynamics of BECs [1, 28]. The most common approach is based on second-quantization formalism for a many-atom system. The field operator \( \Psi (x,t) \) which removes an atom at the location \( x \) at times \( t \) obeys the canonical commutation relations:

\[
\left[ \Psi (x,t) , \Psi (y,t) \right] = 0
\]

\[
\left[ \Psi (x,t) , \Psi^{\dagger} (y,t) \right] = \delta (x - y)
\]

The dynamics of this field is given by the Heisenberg equations of motion

\[- \frac{i \hbar}{\partial t} \Psi = [H, \Psi] \]

where \( H \) is the Hamiltonian

\[
H = \int d^d x \left\{ \Psi H \Psi + \frac{U}{2} (\Psi \Psi)^2 \right\}
\]

\[
H \Psi = - \frac{\hbar^2}{2M} \nabla^2 \Psi + V_{trap} (x) \Psi
\]

and \( V_{trap} (x) \) denotes a confining trap potential. Making the commutator in Eq. explicit we obtain

\[
i \hbar \frac{\partial}{\partial t} \Psi = H \Psi + U \Psi^{\dagger} \Psi^2
\]
The total particle number operator commutes with the Hamiltonian and is therefore conserved. The theory is invariant under a global phase change of the field operator
\[ \Psi \rightarrow e^{i\theta} \Psi, \quad \Psi \rightarrow e^{-i\theta} \Psi \] (7)

B. Problems with the symmetry breaking approach

In the symmetry breaking (SB) approach to BECs, condensation is signaled by the spontaneous breakdown of phase invariance Eq. (7), whereby \( \Psi \) develops a nonzero expectation value \( \Phi \) (c-number). We can therefore employ a background field separation for \( \Psi \) \[1, 2, 30\]
\[ \Psi = \Phi_{SB} + \Psi_q \] (8)

where \( \Psi_q \) (q-number) is the field operator corresponding to quantum fluctuations. Various approaches differ in how to handle the dynamics of these two constituents.

For later reference, we point out that a priori \( \Psi_q \) is not necessarily orthogonal to \( \Phi_{SB} \); also \( \Phi_{SB} \) is not necessarily simply proportional to the condensate wave function as defined below.

A common feature of these approaches is that the total particle number
\[ N = \int d^d x \Psi^\dagger \Psi \] (9)
is not fixed. For example, let us assume that the condensate is confined within a homogeneous box of volume \( V \), condensation occurring in the lowest (translation invariant) mode. Let \( a_\vec{k} \) be the operator that destroys an atom in the \( \vec{k} \) mode. Then we may approximate (see more careful discussion below)
\[ \Psi_q (x, t) = \sum_{\vec{k} \neq 0} e^{i \vec{k} \cdot \vec{x}} \sqrt{V} a_\vec{k} \] (10)

Even if we treat \( \Psi_q \) as a linear perturbation on the condensate, the Hamiltonian is not diagonal on the \( a_\vec{k} \). To diagonalize it, we must introduce phonon destruction operators \( b_\vec{k} \) and perform a Bogolubov transformation
\[ a_\vec{k} = \alpha_k b_\vec{k} + \beta_k b^\dagger_{-\vec{k}} \] (11)

At zero temperature, the state is the phonon vacuum, \( b_\vec{k} |0\rangle = 0 \) for all \( \vec{k} \neq 0 \). We find
\[ \langle N \rangle = \int d^d x \langle \Psi^\dagger \Psi \rangle = V \left[ |\Phi_{SB}|^2 + \tilde{n} \right] \] (12)

where
\[ \tilde{n} = \langle \Psi_q^\dagger \Psi_q \rangle = \frac{1}{V} \sum_{\vec{k} \neq 0} \langle a_{\vec{k}}^\dagger a_\vec{k} \rangle = \frac{1}{V} \sum_{\vec{k} \neq 0} |\beta_k|^2 \] (13)

but
\[ \langle N^2 \rangle = V^2 \left[ (|\Phi_{SB}|^2)^2 + |\Phi_{SB}|^2 \left( 4\tilde{n} + \frac{1}{V} \right) + \Phi_{SB}^* \tilde{m} + \Phi_{SB} \tilde{m}^* + ... \right] \] (14)
where
\[ \tilde{m} = \langle \Psi_\eta^2 \rangle = \frac{1}{V} \sum_{\vec{k} \neq 0} \langle a_\vec{k} a_\vec{k}^\dagger \rangle = \frac{1}{V} \sum_{\vec{k} \neq 0} \alpha_k \beta_k \] (15)

The Bogoliubov coefficients \( \alpha_k \) and \( \beta_k \) cannot be equal, because the canonical (bosonic) commutation relations imply \( |\alpha_k|^2 - |\beta_k|^2 = 1 \), and so also \( \tilde{m} \neq \tilde{n} \). We conclude that necessarily \( \langle N^2 \rangle \neq \langle N \rangle^2 \) in the symmetry breaking approach, signaling the presence of particle number fluctuations.

### C. Particle number conserving functional approach: Global versus local gauge

The Heisenberg equation of motion Eq. (6) is also the classical equation of motion derived from the action
\[ S = \int d^{d+1}x \ i \hbar \Psi^* \frac{\partial}{\partial t} \Psi - \int dt \ H \] (16)

The quantum theory of the BEC may be regarded as the quantization of the nonrelativistic classical field theory defined by the action functional Eq. (16), where the canonical variables are \( \Psi(x,t) \) and its conjugate momentum \( i \hbar \Psi^* \). This theory conserves particle number Eq. (9), and we are interested in the case in which particle number takes on a definite value \( N \). We may reinforce this point by adding a constraint on the theory. This is achieved by introducing a Lagrange multiplier \( \mu_q(t) \), thereby writing the action as
\[ S = \int d^{d+1}x \ \left\{ i \hbar \Psi^* \frac{\partial}{\partial t} \Psi + \hbar \mu_q(t) \left[ \Psi^* \Psi - \frac{N}{V} \right] \right\} - \int dt \ H \] (17)

The original action Eq. (16) is invariant under a global transformation Eq. (7) but the new action Eq. (17) is invariant under the local (in time) transformations (a familiar theory with local U(1) gauge symmetry is electromagnetism)
\[ \Psi \rightarrow e^{i\theta(t)} \Psi, \quad \Psi^\dagger \rightarrow e^{-i\theta(t)} \Psi^\dagger, \quad \mu_q \rightarrow \mu_q + \frac{d\theta}{dt} \] (18)

provided \( \theta \) vanishes both at the initial and final times (when \( \theta \) is infinitesimal, these are just canonical transformations generated by the constraint). Therefore it must be quantized using the methods developed for gauge theories, such as the Fadeev-Popov method (See Appendix B).

In short, the action functionals Eq. (16) and (17) lead to the same classical theories, but to inequivalent quantization schemes. The assertion is that Eq. (17) gives a more complete description of the fundamental theory, as it shows explicitly the gauge dependence while the result of the quantum theory is gauge-invariant. As it has been shown by DeWitt and others, it is possible to introduce an action functional whose variation yields the equations of motion for the expectation values of the fields and preserves the gauge symmetry. The explicit construction of this so-called ”gauge invariant effective action” (GIEA) [31] for the description of BEC dynamics is the subject of this paper.

### D. Specific goals and what are attained

In this paper we shall construct the gauge-invariant effective action (GIEA) for the dynamics of BECs with a fixed total particle number. The variation of this GIEA yields the equations of motion for the background fields.

Since physical description of results depends on the choice of gauge many existing approaches which work within a specific gauge produce results which cannot easily be compared with each other. In the GIEA
approach we can place them in the same framework and be able to compare the similarities and difference in
the physics. For a range of existing theories with particle number conserving constraints \[21, 23, 24, 25, 26\] we show that they are indeed within the same physical theory. Most importantly, the gauge-invariant
formalism provides the necessary foundation to carry on these approaches beyond the next to leading order
approximation in a consistent way. It is in this more ambitious program that the power of the gauge invariant
approach becomes decisive, not optional.

Our goal in this paper is to construct the basic structure for such a program, putting premium emphasis on
the gauge-invariance aspect but limiting our reach only to the “one-particle irreducible” (1PI) level \[32\], as
opposed to a 2PI or Φ- derivable approach \[3\]. The extension to the Φ- derivable formulation (or even further,
to the nPI effective action \[33\]) is necessary to match the accuracy demanded by present day experiments.
A 2PI non-gauge theory description of the nonequilibrium dynamics of BECs is presented in \[13, 14, 17\]; the
2PI approach in gauge theories at large is discussed in \[34\].

Another restriction is that we shall work with the IN-OUT formulation \[32\], as opposed to the closed - time
path (CTP) or Schwinger - Keldysh formulation \[5\]. Beyond the next-to-leading order a truly dynamical
theory requires a CTP formulation which yields real and causal equations of motion \[35\]. Formally, the CTP
dynamical equations may be derived from those in this paper by considering the time variable to be defined
on a closed time path ranging from the distant past to the far future and doubling back to the distant past.
For further discussion we refer the reader to Refs. \[13, 14\].

This paper is organized as follows. In Section II we develop a PNC approach in canonical terms, which
will be later used as a template for the functional approach. Our presentation is close to \[24\], with some
minor technical differences (explained in Appendix A) The essence of the paper is in Section III, where we
construct the GIEA for the description of BECs with a fixed number of particles. We derive the equations
of motion in a large \(N\) expansion, where \(N\) is the number of particles, and show their equivalence to those
derived by canonical methods in Section II, up to NLO. (Observe that in the literature there is also a “large
\(N\)” expansion, where \(N\) is the number of fields \[15, 28\]. These expansions
should not be confused with each other.)

In Section IV we conclude with some brief remarks. Appendix A compares our presentation of the PNC
formalism with those of Girardeau and Arnowitt \[21, 22\], Gardiner \[23\] and Castin and Dum \[24\], and
Appendix B gives a review of gauge field theory quantization and the theory of the GIEA . None of the
material in both Appendices is new, they are added for completeness and easy reference.

II. THE PARTICLE NUMBER CONSERVING FORMALISM

The symmetry-breaking approach described above has the disturbing feature that, strictly speaking, sym-
metry breaking only occurs in the thermodynamic limit. We have therefore a formalism that assumes the
number of particles is essentially infinite. Most actual experiments deal with situations where particle number
is bounded and actually not so large (from a few hundred to a few thousand atoms). Under this circumstance
a condensate as described above simply cannot happen.

In this Section we shall describe an alternative formulation which is designed to deal with gases at a fixed
particle number. We shall call this formulation the particle number conserving formalism, PNC for short. It
was first proposed by Arnowitt and Girardeau \[21\], and it has been extended and improved by many other
people over the last forty years \[22, 23\]. Our own presentation follows Castin and Dum \[24, 26, 27\], with
some minor technical differences which are discussed in Appendix A.

Let us begin by discussing how is it possible to speak of a BEC in a situation where there is no symmetry
breaking.

A. The one-body density matrix and long range coherence

We consider as above a second - quantized Bose field \(\Psi\). The state of the many-body system is an eigenstate
of total particle number operator Eq. \[19\]. There is no particle exchange with the environment.
In this case of a finite system, there is no symmetry breaking. The symmetry broken state is essentially a coherent state and thus a coherent superposition of states with arbitrarily large total particle number. Nevertheless, there are situations where there is long range coherence across the system, thus capturing the essential feature of the condensed states. Sometimes these situations are referred to as quasi-condensates, but we shall not make this distinction, and call them BECs as their symmetry-broken siblings.

To characterize the BEC state, let us introduce the one-body density matrix

\[ \sigma(x, y, t) = \langle \Psi^\dagger(x, t) \Psi(y, t) \rangle \]  

Long range coherence appears when \( \sigma \) fails to decay as \( x \) and \( y \) are taken apart.

Observe that \( \sigma \) is Hermitian and nonnegative, in the sense that for any function \( f \)

\[ \int d^4x d^4y f^*(x) \sigma(x, y, t) f(y) \geq 0 \]  

Therefore it admits a basis of eigenfunctions

\[ \int d^4x \sigma(x, y, t) \phi_\alpha(y, t) = n_\alpha \phi_\alpha(x, t) \]  

where the eigenvalues \( n_\alpha \) are real and nonnegative. We assume the \( \phi_\alpha \) are normalized

\[ (\phi_\alpha, \phi_\beta) = \delta_{\alpha\beta} \]  

\[ (f, g) = \int d^4x f^*g \]  

and complete

\[ \sum_\alpha \phi_\alpha^*(x, t) \phi_\alpha(y, t) = \delta(x - y) \]  

The field operator may be expanded in this basis

\[ \Psi(x, t) = \sum_\alpha a_\alpha(t) \phi_\alpha(x, t) \]  

The Bose commutation relations imply

\[ \left[ a_\alpha(t), a_\beta^\dagger(t) \right] = \delta_{\alpha\beta} \]  

The \( a_\alpha(t) \) are operators which, at time \( t \), destroy a particle in the one-particle state \( \alpha \) whose wavefunction is \( \phi_\alpha(x, t) \). From the definition of \( \sigma \) we find

\[ \langle a_\alpha^\dagger(t) a_\beta(t) \rangle = n_\alpha(t) \delta_{\alpha\beta} \]  

Therefore the eigenvalues \( n_\alpha(t) \) are the mean number of particles in the one-body state \( \alpha \) at time \( t \). We also have the strong identity
\[ N = \sum_{\alpha} a_{\alpha}^\dagger (t) a_\alpha (t) \tag{28} \]

Condensation occurs when one of the \( n_\alpha \), say \( \alpha = 0 \), becomes comparable with \( N \) itself. Then we have, for large separations

\[ \sigma (x, y, t) \sim n_0 \phi_0^* (x, t) \phi_0 (y, t) \tag{29} \]

which displays long range coherence, as expected. Here \( \phi_0 (x, t) \) is the condensate wave function. We must stress that this is the fundamental definition; \( \phi_0 (x, t) \) is not necessarily identical to the mean field \( \Phi_{SB} \) introduced in the symmetry-breaking approach (for one, \( \Phi_{SB} \) is not normalized).

**B. The dynamics of the condensate wave function**

We shall now discuss the dynamics of the condensate wave function \( \phi_0 (x, t) \) and the condensate occupation number \( N_0 \) (we switch to a capital \( N \) to emphasize its macroscopic character). We envisage a situation in which \( N \) is finite but large, and will seek equations of motion as an expansion in inverse powers of \( N \). In preparation for this, it is convenient to scale the interaction term, writing \( U = u/N \).

The idea is to exploit the fact that \( a_0 \) is “large” and the other destruction operators are not. Let us define new operators \( \lambda_\alpha, \alpha \neq 0 \), through

\[ a_\alpha \equiv a_0 \frac{1}{\sqrt{N}} \lambda_\alpha \tag{30} \]

The \( \lambda_\alpha \) do not commute with \( a_0^\dagger \)

\[ a_0 \left[ \lambda_\alpha, a_0^\dagger \right] + \lambda_\alpha = 0 \tag{31} \]

but they commute with \( N \). Let us define the non-condensate field

\[ \Lambda (x, t) = \sum_{\beta \neq 0} \lambda_\beta (t) \phi_\beta (x, t) \tag{32} \]

so the Heisenberg field operator becomes

\[ \Psi (x, t) = a_0 (t) \left[ \phi_0 (x, t) + \frac{1}{\sqrt{N}} \Lambda (x, t) \right] \tag{33} \]

we have the identities

\[ (\phi_0, \Lambda) = 0 \tag{34} \]

\[ \langle a_0^\dagger a_0 \Lambda (x, t) \rangle = 0 \tag{35} \]

The condensate occupation number is
\[ N_0 = N \left[ 1 - \frac{\nu}{N} + o \left( N^{-1} \right) \right] \]  

(36)

\[ \nu = \sum_{\beta \neq 0} \lambda_{\beta}^\dagger \lambda_{\beta} \]  

(37)

We seek a solution of the Heisenberg equations of motion Eq. (6) of the form

\[ a_0 = \sqrt{N} e^{-i\Theta(t)} \left[ \gamma + \frac{\gamma_1}{N^{1/2}} + \frac{\Delta \gamma}{N} \right] \]  

(38)

\[ \phi_0 = \Phi + \frac{\Delta \Phi}{N} \]  

(39)

\[ \Lambda = \Lambda_0 + \frac{\Delta \Lambda}{N^{1/2}} \]  

(40)

where \( \gamma \) is a constant q-number and \( \gamma^\dagger \gamma = \gamma \gamma^\dagger = 1 \). Expanding the canonical commutation relations we get

\[ \left[ \gamma, \gamma_1^\dagger \right] + \left[ \gamma_1^\dagger, \gamma \right] = \left[ \Lambda_0, \gamma^\dagger \right] = 0 \]  

(41)

\[ \left[ \gamma_1^\dagger, \gamma_1^\dagger \right] + \left[ \gamma, \Delta \gamma^\dagger \right] + \left[ \Delta \gamma, \gamma^\dagger \right] = 1 \]  

(42)

The expansion of the Heisenberg equations in inverse powers of \( N \) yields at leading order the Gross-Pitaevsky equation (GPE) for \( \Phi \)

\[ 0 = i \frac{\partial \Phi}{\partial t} - H \Phi - u \Phi^* \Phi^2 + \mu \Phi \]  

(43)

with a possibly time-dependent chemical potential

\[ \mu = \frac{d\Theta}{dt} \]  

(44)

The actual value of \( \mu \) is derived by consistency with the normalization of \( \Phi \). The next-to-leading order (NLO) terms read

\[ 0 = i \gamma^\dagger \frac{d\gamma_1}{dt} \Phi + i \frac{\partial \Lambda_0}{\partial t} - H \Lambda_0 - u \left[ \left( 2 \Phi^* \Phi - \frac{\mu}{u} \right) \Lambda_0 + \Phi^2 \Lambda_0^\dagger \right] \]  

(45)

Projecting over \( \Phi \) we get

\[ 0 = i \gamma^\dagger \frac{d\gamma_1}{dt} - \left( \Phi, u \left[ \Phi^* \Phi \Lambda_0 + \Phi^2 \Lambda_0^\dagger \right] \right) \]  

(46)
and finally

\[ 0 = i \frac{\partial \Lambda_0}{\partial t} - H \Lambda_0 - u (\Phi^* \Phi) \Lambda_0 + \mu \Lambda_0 - uQ \left[ \Phi^* \Phi \Lambda_0 + \Phi^2 \Lambda_0 \right] \]  

(47)

where

\[ Q[f] = f - \Phi (\Phi, f) \]  

(48)

Observe that the equation for \( \gamma_1 \) is consistent with the requirement that \( N_0/N = 1 - O(N^{-1}) \), since

\[ \frac{d}{dt} \left[ \gamma_1 \gamma_1^\dagger + \gamma_1^\dagger \gamma_1 \right] = 0 \]  

(49)

so we may impose the condition \( \gamma_1 \gamma_1^\dagger + \gamma_1^\dagger \gamma_1 = 0 \).

We see that these equations do not determine \( \gamma \). Since the one body density matrix is independent of it, \( \gamma \) may be chosen freely. The simplest choice is \( \gamma = 1 \), in which case Eq. (42) reduces to

\[ \left[ \gamma_1, \gamma_1^\dagger \right] = 1 \quad (\gamma = 1) \]  

(50)

With this choice, the requirement that \( \gamma_1 + \gamma_1^\dagger = 0 \) must be understood as a restriction on the allowed states, rather than as a strong identity, since it would conflict with Eq. (50). We shall discuss this issue in more detail in the next section.

III. GAUGE INVARIANT EFFECTIVE ACTION FOR BOSE-EINSTEIN CONDENSATES

Consider the vacuum persistence amplitude for a theory with classical action \( S \) as in Eq. (16), expressed as a path integral over paths with total particle number \( N \)

\[ Z_0 = \int D\Psi e^{iS/\hbar} \prod_t \delta \left( \int d^d x \Psi^\dagger \Psi \right) - N \].  

(51)

Exponentiate the delta functions

\[ Z_0 = \int D\Psi D\mu_q e^{iS_\mu/\hbar} \]  

(52)

\[ S_\mu = S + \hbar \int d^{d+1} x \mu_q(t) \left[ \Psi^\dagger \Psi - \frac{N}{V} \right] \]  

(53)

Observe that now the path integral is redundant, since we may transform the fields as in Eq. (18). We may fix the redundancy by factoring out the gauge group. Choose some function \( f_\theta = f \left[ \mu_\theta, \Psi_\theta, \Psi_\theta^\dagger \right] \), such that \( df_\theta/d\theta \neq 0 \). Then

\[ 1 = \int \frac{df_\theta}{df_\theta} d\theta \delta (f_\theta - c) \]  

(54)
Inserting this into the vacuum persistence amplitude and average over \( c \) with a weight \( e^{ic^2/2\sigma} \) we get

\[
Z_0 = \Theta \int D\Psi D\mu_q e^{iS_{\mu,\sigma}}/h \text{Det} \left[ \frac{\delta f_0}{\delta \theta} \right]_{\theta=0}
\]  

(55)

where

\[
\Theta = \int D\theta
\]  

(56)

is the volume of the gauge group we wish to factor out.

\[
S_{\mu,\sigma} = S + \hbar \int d^{d+1}x \mu_q(t) \left[ \Psi^\dagger \Psi - \frac{N}{V} \right] + \frac{\hbar}{2\sigma} \int dt f_0^2
\]  

(57)

The determinant is expressed as a path integral over Grassmann fields \( \zeta, \eta \)

\[
\text{Det} \left[ \frac{\delta f_0}{\delta \theta} \right]_{\theta=0} = \int D\zeta D\eta e^{\frac{1}{\hbar} \int dt \zeta \frac{\delta f_0}{\delta \theta} \eta}
\]  

(58)

Thus, we have a theory of fields \( \Psi, \Psi^\dagger, \mu_q, \zeta \) and \( \eta \). Suppose we wish now to compute the one loop effective action for this theory. We redefine \( \Psi = \bar{\Phi} + \Psi_q \) as in Eq. (8). Similarly redefine \( \Psi^\dagger = \bar{\Phi}^* + \Psi_q^\dagger \), and \( \mu_q = \bar{\mu}_q + \lambda \). Doing so introduces an undesirable cross term

\[
\hbar \int d^{d+1}x \lambda(t) \left[ \bar{\Phi}^* \Psi_q + \bar{\Phi} \Psi_q^\dagger \right]
\]  

(59)

To eliminate this term, we choose

\[
f = -\sigma(\mu_q - \bar{\mu}_q) + \int d^dx \left[ \Phi^*\bar{\Psi}^\dagger + \bar{\Phi}^*\Psi^\dagger - 2|\Phi|^2 \right]
\]  

(60)

The ghost action now becomes

\[
S_{\text{ghost}} = i \int dt \zeta \left[ -\sigma \frac{d}{dt} + \int d^dx \left( \bar{\Phi}^*\Psi_q - \bar{\Phi}\Psi_q^\dagger \right) \right] \eta
\]  

(61)

and it decouples at one-loop order.

**A. Inverse particle number as a small parameter**

The loop expansion is a formal development in which Feynman graphs are classified according to their topology. This has strong heuristic value but is hard to estimate a priori which order in perturbation theory must be reached to guarantee any prescribed accuracy. The inverse of the total particle number \( N \) provides a small parameter with a clear physical meaning, and so it is convenient to organize the perturbative expansion as a development in inverse powers of \( N \). As we shall see, this may be achieved through a Stratonovich transformation of the interaction term.

Let us begin by rewriting the classical action as (from now on, we assume \( \hbar = 1 \))
\[ S_N = \int dt d^d x \left\{ i \Psi^\dagger D_t \Psi - \Psi^\dagger H \Psi - \frac{u}{2N} \Psi^1 \Psi^2 \right\} \] (62)

with \( \mu_q \) as connection in the covariant derivative

\[ D_t = \frac{\partial}{\partial t} - i \mu_q \] (63)

We have assumed the nonlinear term scales with \( N \) in a particular way \((U \rightarrow u/N)\) to make sure the large \( N \) limit is well defined.

We add a term

\[ \frac{u}{2N} \int dt d^d x \left( \Psi_{12} - \frac{N}{u} \Omega^\dagger \right) \left( \Psi^2 - \frac{N}{u} \Omega \right) \] (64)

to the action, whose only effect is to multiply the generating functional by a constant factor, and integrate over the new auxiliary fields \( \Omega \) and \( \Omega^\dagger \). The action now reads

\[ S_N = \int dt d^d x \left\{ i \Psi^\dagger D_t \Psi - \Psi^\dagger H \Psi - \frac{1}{2} (\Omega^\dagger \Psi^2 + \Psi^1 \Omega) + \frac{N}{2u} \Omega^\dagger \Omega - \frac{N}{V} \right\} \] (65)

We add to this action the gauge fixing term as in Eq. (57). The gauge fixing condition is given by Eq. (60), where the gauge parameter is chosen to be \( \sigma = Ns \), and the ghost term Eq. (61).

Finally we rescale \( \Phi = \sqrt{N} \phi, \Phi^* = \sqrt{N} \phi^* \) and \( \Psi_q = \sqrt{N} \psi, \Psi_q^\dagger = \sqrt{N} \psi^\dagger \), whereby we get

\[ \Psi = \sqrt{N} \left[ \phi + \psi \right] \] (66)

\[ S_N \left[ \Psi, \Omega, \mu_q, \zeta, \eta, \Phi \right] = N S_1 \left[ \phi + \psi, \Omega, \mu_q, \zeta, \eta, \phi \right] \] (67)

Henceforth, we shall write \( S_1 \equiv S \).

In the rescaled theory there are only cubic interactions; all vertices scale like \( N \), and all propagators scale as \( N^{-1} \). It follows that the power of \( N \) for any given graph is simply \( 1 - \ell \), where \( \ell \) is the number of loops.

### B. Leading order equations of motion

Introduce background fields \( \bar{\Omega} \) and \( \bar{\mu}_q \) for the fields \( \Omega = \bar{\Omega} + \omega, \mu_q = \bar{\mu}_q + \lambda \). To leading order in \( N \), the theory reduces to the classical one, with equations of motion

\[ i D_t \phi - H \phi - \bar{\Omega} \phi^* = 0 \] (68)

\[ \int d^d x \phi^* \phi = 1 \] (69)

\[ \phi^2 - \frac{\bar{\Omega}}{u} = 0 \] (70)
where $\bar{D} \equiv \partial_t - i\bar{\mu}_q$ is the covariant derivative evaluated with $\bar{\mu}_q$ as connection. To make contact with the PNC formalism above, we assume (cfr. Eqs. (38) and (39))

$$\phi = e^{-i\Theta(t)} \left[ \Phi + \frac{\Delta\phi}{N} \right]$$

and $\bar{\mu}_q = 0$. We therefore get the GPE Eq. (43) for $\Phi$, with $\mu = d\Theta/dt$ as in Eq. (44) above.

### C. The fluctuation fields at leading order

To compute the first order corrections, namely, terms of order $N^0$ in the effective action, we must keep quadratic terms in the fluctuations, namely

$$S_N [\Psi, \Omega, \mu_q, \zeta, \eta, \Phi] = NS [\phi, \bar{\Omega}, \bar{\mu}_q, \zeta, \eta, \phi] + NS_{\text{quad}}$$

$$S_{\text{quad}} = \int dt d^d x \left\{ i\tilde{\psi}^\dagger \bar{D}_t \tilde{\psi} - \tilde{\psi}^\dagger H\tilde{\psi} - \frac{1}{2} \left[ \bar{\Omega}^\dagger \tilde{\psi}^2 + \tilde{\psi}^\dagger \bar{\Omega}^\dagger \right] - 2u\phi^\dagger \phi \tilde{\psi}^\dagger \tilde{\psi} + \frac{1}{2u} \bar{\Omega}^\dagger \bar{\psi}^\dagger \Omega + \frac{1}{2} \bar{\Omega}^\dagger \bar{\psi}^\dagger \Omega = 0 \right\}$$

The ghost and gauge action decouple to lowest order, but they must be included at higher orders. To eliminate the $\omega \tilde{\psi}$ cross terms, we redefine

$$\omega = \varpi + 2u\phi \tilde{\psi}$$

and get

$$S_{\text{quad}} = \int dt d^d x \left\{ i\tilde{\psi}^\dagger \bar{D}_t \tilde{\psi} - \tilde{\psi}^\dagger H\tilde{\psi} - \frac{1}{2} \left[ \bar{\Omega}^\dagger \tilde{\psi}^2 + \tilde{\psi}^\dagger \bar{\Omega}^\dagger \right] - 2u\phi^\dagger \phi \tilde{\psi}^\dagger \tilde{\psi} + \frac{1}{2} \bar{\Omega}^\dagger \bar{\psi}^\dagger \Omega = 0 \right\}$$

The $\varpi, \lambda$ and the ghost fields are decoupled and play no further role at NLO. Making one last scaling and a phase shift

$$\tilde{\psi} = N^{-1/2} e^{-i\Theta(t)} \psi,$$

we find that to leading order the field $\psi$ is a quantized linear field obeying the Heisenberg equation of motion

$$iD_t \psi - H\psi - u\Phi^2 \psi^\dagger - 2u\Phi^\dagger \Phi \psi = \frac{\Phi}{s} \int d^d y \left[ \Phi^\dagger \psi + \psi^\dagger \Phi \right] (y, t)$$

and commutation relations

$$[\psi(x,t), \psi^\dagger(y,t)] = \delta(x-y)$$
We have assumed $\bar{\mu}_q = 0$; $D_t \equiv \frac{\partial}{\partial t} - i\mu$ is the covariant derivative with $\mu$ as connection.

Let us split the fluctuation field into its components along the mean field (longitudinal) and orthogonal to it (transverse)

$$\psi(x, t) = \psi_0(t) \Phi(x, t) + \psi_\perp(x, t)$$  \hspace{1cm} (79)

where $\psi_0 = (\Phi, \psi)$ and $\psi_\perp = Q\psi$ (cfr. Eq. (48)). The ETCCR imply

$$\left[\psi_0, \psi_0^\dagger\right] = 1$$  \hspace{1cm} (80)

$$\left[\psi_0, \psi_\perp^\dagger\right] = 0$$  \hspace{1cm} (81)

$$\left[\psi_\perp(x, t), \psi_\perp^\dagger(y, t)\right] = Q\delta(x - y)$$  \hspace{1cm} (82)

We substitute Eq. (79) into the wave equation for the fluctuations Eq. (77); using also the GPE Eq. (43)

$$0 = i\frac{d\psi_0}{dt} \Phi + A \left[\psi_0 + \psi_0^\dagger\right] - C \left[\psi_\perp\right]$$  \hspace{1cm} (83)

where

$$A = \Phi s - u\Phi^*\Phi^2$$  \hspace{1cm} (84)

$$C \left[\psi_\perp\right] = -iD_t\psi_\perp + H\psi_\perp + u\Phi^2\psi_\perp^\dagger + 2u\Phi^*\Phi^2\psi_\perp$$  \hspace{1cm} (85)

Projecting over $\Phi$ we get the equation for the longitudinal mode

$$i\frac{d\psi_0}{dt} + A_0 \left[\psi_0 + \psi_0^\dagger\right] = C_0 \left[\psi_\perp\right]$$  \hspace{1cm} (86)

where

$$A_0 = (\Phi, A)$$  \hspace{1cm} (87)

$$C_0 \left[\psi_\perp\right] = (\Phi, C \left[\psi_\perp\right]) = u \left(\Phi, \left[\Phi^2\psi_\perp^\dagger + \Phi^*\Phi^2\psi_\perp\right]\right)$$  \hspace{1cm} (88)

Now observe that both $A_0$ and $C_0 \left[\psi_\perp\right]$ are real, so writing

$$\psi_0 = \xi + i\eta$$  \hspace{1cm} (89)

with ETCCR
\[ [\xi, \eta] = \frac{i}{2} \]

we get

\[ \frac{d\xi}{dt} = 0 \]  \hspace{1cm} (91)

\[ \frac{d\eta}{dt} = 2A_0\xi - C_0[\psi_\bot] \]  \hspace{1cm} (92)

We realize that Eq. (91) is the counterpart to Eq. (49), so to match the GIEA and PNC approaches we set \( \xi = 0 \). Comparing Eq. (92) to Eq. (46), we see that the longitudinal fluctuation field is simply \( \psi_0 = \gamma_1 \), where the choice \( \gamma = 1 \) has been made. As discussed in the last section, we do not regard \( \xi = 0 \) as a strong condition, but rather as a restriction on allowed physical states. We shall discuss this issue in the next subsection.

The equation for the orthogonal component \( \psi_\bot \) is now

\[ QC[\psi_\bot] = C[\psi_\bot] - \Phi C_0[\psi_\bot] = 0 \]  \hspace{1cm} (93)

where \( C \) and \( C_0 \) are defined in Eqs. 85 and 88, respectively. Since this is equivalent to Eq. 47, we identify \( \psi_\bot = \Lambda_0 \).

D. Gauge fixing dependence of the two point functions

To complete the evaluation of the next-to-leading order (NLO) corrections to the mean fields and the one-body density matrix, we need the LO two point functions of the theory, that is, the expectation values of the products of two fluctuation fields. In this subsection we shall discuss the important issue of whether these two-point functions are gauge-fixing dependent, that is, whether they depend on the parameter \( s \). Of course, physical observables, the one-body density matrix among them, must be gauge fixing independent.

Observe that \( s \) has disappeared from the Heisenberg equation for \( \psi_\bot \) Eq. (93), so the two point functions built from it are automatically gauge fixing independent. As for the two point functions involving the longitudinal modes \( \xi \) and \( \eta \), we translate the requirement \( \xi = 0 \) into

\[ \langle \xi^2 \rangle = \langle \xi \eta + \eta \xi \rangle = 0 \]  \hspace{1cm} (94)

while the ETCCR means

\[ \langle \xi \eta - \eta \xi \rangle = \frac{i}{2} \]  \hspace{1cm} (95)

Eq. 84 implies

\[ \frac{d}{dt} \langle \eta(t) \psi_\bot(y, t') \rangle = -C_0[\langle \psi_\bot(, t) \psi_\bot(y, t') \rangle] \]  \hspace{1cm} (96)

We see that there are nontrivial correlations between the longitudinal and the transverse quantum field, but they are gauge fixing independent.

Finally
\[
\frac{d}{dt} \langle \eta(t) \eta(t') \rangle = i A_0(t) - C_0 \langle \psi_\perp(t) \eta(t') \rangle
\]  
(97)

\[
\frac{d}{dt} \langle \eta(t) \eta(t') \rangle = -i A_0(t') - C_0 \langle \eta(t) \psi_\perp(t) \rangle
\]  
(98)

These two equations show that we may write

\[
\langle \eta(t) \eta(t') \rangle = \langle \eta(t) \eta(t') \rangle_0 + \frac{i}{2} \int_{t'}^t d\tau A_0(\tau)
\]  
(99)

where \( \langle \eta(t) \eta(t') \rangle_0 \) is gauge fixing independent. In particular, the gauge fixing dependence disappears in the coincidence limit \( t' = t \).

We may now proceed to evaluate the NLO mean fields.

**E. The mean fields at next to leading order**

We may write the GIEA to one loop order as

\[
\Gamma_{GI} [\phi, \bar{\mu}, \bar{\Omega}] = NS [\phi, \bar{\Omega}, \bar{\mu}_q, 0, 0, \phi] + \Gamma_1 [\phi, \bar{\mu}_q, \bar{\Omega}]
\]  
(100)

\[
\Gamma_1 = -i \ln \left[ \int D\psi D\psi^\dagger e^{iS_{quad}[\psi, \psi^\dagger]} \right]
\]  
(101)

To NLO we write the mean fields as

\[
\phi = e^{-i\Theta(t)} \left[ \Phi + \frac{\phi^{(1)}}{N} + o(N^{-1}) \right]
\]  
(102)

\[
\bar{\Omega} = e^{-2i\Theta(t)} \left[ u\Phi^2 + \frac{\bar{\Omega}^{(1)}}{N} + o(N^{-1}) \right]
\]  
(103)

\[
\bar{\mu}_q = \frac{\mu^{(1)}}{N}
\]  
(104)

We also split \( \phi^{(1)} \) into components along the LO mean field (longitudinal) and perpendicular to it (transverse)

\[
\phi^{(1)} = \phi^{(1)}_0 \Phi + \phi^{(1)}_\perp
\]  
(105)

The equations of motion for the NLO terms become

\[
0 = i D_t \phi^{(1)} - H \phi^{(1)} - u \Phi^2 \phi^{(1)*} - \bar{\Omega}^{(1)} \Phi^* - 2u \langle \psi^\dagger \psi \rangle \Phi \\
+ \frac{1}{s} \langle \psi_0(t) \Phi(x,t) + \psi_\perp(x,t,\xi) \rangle + \mu^{(1)} \Phi
\]  
(106)
\[ \phi_0^{(1)} + \phi_0^{(1)*} + \langle \psi_0^\dagger \psi_0 \rangle + \nu = 0 \]  

(107)

\[ \Phi \left( 2\phi^{(1)} + \langle \{ \psi_0, \psi_\perp \} \rangle \right) + \langle \psi_0^2 \rangle \Phi^2 + \langle \psi_\perp^2 \rangle - \frac{\bar{\Omega}^{(1)}}{\nu} = 0 \]

(108)

where we identified \( \psi_\perp = \Lambda_0 \) and introduced \( \nu \) from Eq. (37).

In view of the analysis in the previous subsection, the explicitly \( s \)-dependent term in Eq. (106) vanishes. All other two-point functions are in the coincidence limit, and so they are gauge fixing independent. We may conclude that the NLO correction to the mean fields themselves is gauge fixing independent. This is the only property of these corrections we shall need in the remainder.

F. The one-body density matrix at next to leading order

From the analysis above, we see that in the GIEA approach we obtain the Heisenberg field operator for the bosonic field as

\[ \Psi = \sqrt{N} e^{-i\Theta(t)} \left\{ 1 + \frac{\psi_0}{\sqrt{N}} + \frac{\phi_0^{(1)}}{\sqrt{N}} \right\} \Phi + \frac{\psi_\perp}{\sqrt{N}} + \frac{\phi_\perp^{(1)}}{\sqrt{N}} \}

(109)

Observe that this is also the result of the canonical PNC approach Eq. (33) under the choice \( \gamma = 1 \). Since it is observable, \( \sigma_m \) must be explicitly gauge independent.

We get, using the NLO equations of motion Eq. (107),

\[ \sigma_m (x,y) = \sigma_0 (x,y) + \delta \sigma_m (x,y) \]

(110)

\[ \sigma_0 (x,y) = N \Phi^* (x) \Phi (y) \left[ 1 - \frac{\nu}{N} \right] \]

(111)

\[ \delta \sigma_m (x,y) = \Phi^* (x) \left( \phi_\perp^{(1)} (y) + \langle \psi_\perp^\dagger \psi_\perp (y) \rangle \right) \]

\[ + \left( \phi_\perp^{(1)*} (x) + \langle \psi_\perp^\dagger (x) \psi_0 \rangle \right) \Phi (y) + \langle \psi_\perp^\dagger (x) \psi_\perp (y) \rangle \]

(112)

To diagonalize this, we simply think of \( \delta \sigma_m \) as a perturbation of \( \sigma_0 \). \( \sigma_0 \) clearly admits \( \Phi \) as an eigenvector with eigenvalue \( N - \nu \). Since \( (\Phi, \delta \sigma_m \Phi) = 0 \), there is no correction to this eigenvalue at first order. This means that the condensate occupation number is \( N_0 = N \left[ 1 - \nu/N + o \left( N^{-1} \right) \right] \), as in the canonical approach, Eq. (36). The actual condensate wave function is

\[ \phi_0 = \Phi + \frac{1}{N} \left( \phi_\perp^{(1)} (y) + \langle \psi_0^\dagger \psi_\perp (y) \rangle \right) \]

(113)

which is not the same as the NLO mean field. Both the condensate occupation number and wave function are explicitly gauge independent, as expected.

Finally we mention that, in spite of there being nontrivial mean fields, the expectation value of the bosonic field operators is zero, as it must be in a finite system. This comes about because the field operator transforms a physical state into one that does not satisfy the particle number constraint; for further discussion, see [39].
We have presented a functional formulation for cold atomic gases. This condition enters as a constraint in the path integral, thus changing the global $U(1)$ symmetry of the model to a local (in time) one. Therefore the theory must be quantized by the Fadeev - Popov method. We derived a gauge-invariant effective action for the description of its dynamics.

To make contact with the more familiar approaches, we draw attention to the fact that the mean field is not necessarily identical with the condensate wave function. However, once the mean field is found, it is easy to obtain the condensate wave function as an expansion in inverse powers of particle number.

The approach presented in this paper unveils the physical equivalence of several proposals in the literature, which now can be seen as different gauge (and gauge fixing condition) choices within the same theory. Thus, if one takes the $s \to \infty$ limit, one eliminates the fluctuations in the self-consistent, time-dependent chemical potential $\mu$ and the ghost field, but places no restriction on quantum fluctuations of the atomic field in the condensate mode. This is the road taken in [37] and [13]. In the opposite $s \to 0$ limit one forces quantum fluctuations in the condensate mode to vanish, but must include chemical potential and ghost fluctuations in higher order perturbation theory. As we can see, neither of these alternatives is the best in every conceivable situation, which testifies to the value of a general formalism as presented here. The other gain in this approach is of course to make contact with the extensive body of work on gauge theories.

The more general nature of this new (gauge invariant) approach is the appearance of a new parameter $s$. While explicitly present in the intermediate steps it does not appear in the final result, as physical predictions should not depend on it (gauge-fixing independence). As there is considerable expertise in identifying the physically relevant, $s$-independent predictions of the theory, this is a lesser evil than its appearance suggests [38]. After all this is as old a topic as electromagnetism, told in the modern gauge theory language.

As a first concrete application, in [39] the functional PNC approach is used to study the one-body density matrix for a cold bosonic gas in an optical lattice, near the superfluid - insulator transition. In this application yet another gauge choice is made (in gauge theory parlance, a simpler “covariant” gauge as opposed to the “background field” gauges used here). This reflects on the flexibility of the method to adapt to the challenges of a concrete environment, knowing that physical equivalence is guaranteed throughout by general theorems.

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APPENDIX A: BRIEF SURVEY OF PNC PROPOSALS

In this Appendix, we shall compare in some detail the PNC formalism presented in Section II with those of [21, 23, 24]. We proceed in chronological order of publication.

1. The Girardeau - Arnowitt theory

The Girardeau - Arnowitt (GA) theory [21] stands apart from the other two proposals to be discussed because its goal is to characterize the BEC ground state within a variational approximation, rather than a dynamical theory. Only the homogeneous case is discussed, so linear momentum is a good quantum number for one-particle states. Finally, GA do not perform a large N expansion; they aim to describe the BEC regime even when depletion is large.

The basic insight of the GA theory is that in the Bogoliubov theory the ground state is seen as a coherent superposition of states with different numbers of particle pairs (a particle of momentum \( p \) correlated to one of momentum \(-p\)) and thus different total particle numbers (see any textbook presentation, e. g. [40]). GA describe the ground state as a coherent superposition of particle - hole pairs (a particle of momentum \( p \), another one of momentum \(-p\), and two particles less in the condensate), all of them having the same total particle number. A particle - hole is destroyed by the operator \( c_p = a_p \beta_0 \) [22], where \( a_p \) destroys a particle of momentum \( p \) and

\[
\beta_0 = (N_0 + 1)^{-1/2} a_0
\]

where we follow the updated formulation of [22]. In terms of the notation of Section II, Eqs. (38), (39), and (40) we have (we assume \( \gamma = 1 \))

\[
\beta_0 = \sqrt{\frac{N}{N_0 + 1} e^{-i\Theta(t)}} \left[ 1 + \frac{\gamma_1}{N^{1/2}} + \frac{\Delta N}{N} \right]
\]

\[
\sim e^{-i\Theta(t)} \left[ 1 + \frac{\gamma_1}{N^{1/2}} + \frac{\Delta N}{N} \right] \quad (A2)
\]

From Eq. (30), the particle - hole destruction operator is

\[
c_p = \frac{1}{\sqrt{N}} \lambda_p N_0 (N_0 + 1)^{-1/2}
\]

\[
= \lambda_p \sqrt{\frac{N}{N_0 + 1}} \sim \lambda_p + O\left(N^{-1}\right) \quad (A3)
\]

In the homogeneous case \( \Phi = \phi_0 = 1/\sqrt{V} \). Therefore Eq. (46) gives \( \gamma_1 = \text{constant} \), the Gross - Pitaevsky equation (43) yields \( \mu = u/V \) and Eq. (47) becomes

\[
0 = i\frac{\partial \lambda_p}{\partial t} - \frac{p^2}{2m} \lambda_p - \frac{u}{V} [\lambda_p + \lambda_p^\dagger] \quad (A4)
\]

which also follows from the GA Hamiltonian at leading order (see Eq. (14) in [22]).

These formulae provide the translation between the GA theory and our formalism.
2. The Gardiner theory

Gardiner’s theory is also a systematic large \( N \) expansion of the Heisenberg equations of motion, after introducing an ansatz equivalent to Eq. for the field operator. The condensate wave function is not introduced as an eigenfunction of the one-body density matrix, but rather kept as an unknown. The Gross - Pitaevsky equation Eq. is derived as a consistency condition, because if it does not hold, then the time derivative of the non-condensate field acquires a term of order \( N^{1/2} \), thus invalidating the large \( N \) expansion. This procedure is sufficient for a NLO discussion as carried out in this paper, but the condensate - non condensate separation becomes ambiguous at higher orders, in which case the Castin and Dum proposal may be preferable.

3. The Castin and Dum theory

As we have stated in the Introduction, our presentation of the PNC method in Section II follows the Castin and Dum theory. The only difference is that Castin and Dum define the non-condensate operator as (in the notation of Section II)

\[
\Lambda_{\text{ex}}(x,t) = N_0 N \Lambda(x,t) \tag{A5}
\]

This makes Eq. simpler

\[
\langle \Lambda_{\text{ex}}(x,t) \rangle = 0 \tag{A6}
\]

allowing for a clearcut separation between the condensate and noncondensate contributions to the equations of motion, but the expression of the Heisenberg field in terms of \( \Lambda_{\text{ex}}(x,t) \) is more involved than in terms of \( \Lambda(x,t) \). Otherwise, both formulations are fully equivalent.

For further developments within the PNC formulation, see [26, 27].

APPENDIX B: THE GAUGE INVARIANT EFFECTIVE ACTION

In this section, we shall review the theory of the GIEA. We begin by introducing the effective action in a general non-gauge theory.

1. The effective action

Consider a theory of fields \( \Psi^i \) whose dynamics is described by an action \( S[\Psi^i] \). The evolution of the fields from some initial to some final times (usually minus and plus infinity, respectively) can be represented by the vacuum persistence amplitude defined as the amplitude for the initial vacuum state to evolve into the OUT vacuum state:

\[
Z[0] = \langle 0_{\text{out}} | 0_{\text{in}} \rangle = e^{iW[0]} = \int D\Psi^i e^{iS[\Psi^i]} \tag{B1}
\]

where we set \( \hbar = 1 \) and adopt the DeWitt convention that a single index \( i \) denotes both space-time and internal indices, and repeated indices denote integration over space-time and summation over internal indices. More general initial and final states may be considered, but this shall be enough for our purposes.

If we allow the fields to interact with external c-number sources \( J_i \), then the persistence amplitude becomes the generating functional. Its Legendre transform is the effective action, which obeys
Consider fluctuations $\psi^i$ around the background fields $\Phi^i$ with $\Psi^i = \Phi^i + \psi^i$, and expand the action for $\psi^i$ to second order in $\psi^i$:

$$S[\Phi + \psi] \sim S[\Phi] + S,[\psi] + \frac{1}{2} S,ij \psi^i \psi^j$$

Then

$$\Gamma[\Phi] = S[\Phi] + \delta \Gamma$$

where

$$e^{i\delta \Gamma[\Phi]} = \int D\psi^i e^{i\left(S[\psi] - \Gamma,_{i}(\psi^i - \Phi^i)\right)}$$

To leading order, $\delta \Gamma,i$ on the right hand side may be neglected, then the one-loop effective action is given by

$$\delta \Gamma = \frac{i}{2} \ln \Det [S,ij]^{-1}$$

2. The effective action for gauge theories \[42, 43\]

Let us consider now the case where the classical action is invariant under an infinitesimal gauge transformations parametrized by $\varepsilon^\alpha$

$$\Psi^i \rightarrow \Psi^i [\varepsilon] = \Psi^i + \delta \Psi^i$$

$$\delta \Psi^i = Q^i_{\alpha} [\Psi^i] \varepsilon^\alpha$$

$$S,iQ^i_{\alpha} = 0.$$  \hspace{1cm} (B10)

We assume the gauge transformations are linear

$$Q^i_{\alpha,jk} = 0,$$  \hspace{1cm} (B11)

that they form a group.
\[ Q_{\alpha,j}^{i} - Q_{\beta,j}^{i} = C_{\alpha\beta}^{\gamma} Q_{\gamma}^{i} \]  

(B12)

and are volume-preserving

\[ Q_{\alpha,i}^{i} = 0 \]  

(B13)

The structure constants satisfy the Jacobi identity and

\[ C_{\alpha\beta}^{\alpha} = 0 \]  

(B14)

Our previous definition of the persistence amplitude is inadequate because gauge equivalent configurations are counted as distinct. To obtain a satisfactory definition we must modify the measure of integration in such a way that each gauge orbit is counted only once.

Let us introduce linear functions \( f_{\alpha}^{i} \) which are not gauge invariant; in particular, we request

\[ \Delta_{\beta}^{\alpha} = f_{\beta}^{j} Q_{\beta}^{j} \]  

(B15)

to have an inverse. Then

\[
\int D\epsilon^{\alpha} \text{Det} \left[ \Delta_{\beta}^{\alpha} \left[ \Psi^{i} \left[ \epsilon \right] \right] \right] \delta \left[ f^{\alpha} \left[ \Psi^{i} \left[ \epsilon \right] \right] - c^{\alpha} \right] e^{iS \left[ \Psi^{i} \right]} = 1
\]  

(provided the argument of the delta functions vanishes somewhere), and we may write

\[
Z \left[ 0 \right] = \int D\epsilon^{\alpha} \int D\Psi^{i} \text{Det} \left[ \Delta_{\beta}^{\alpha} \left[ \Psi^{i} \left[ \epsilon \right] \right] \right] \delta \left[ f^{\alpha} \left[ \Psi^{i} \left[ \epsilon \right] \right] - c^{\alpha} \right] e^{iS \left[ \Psi^{i} \right]}
\]  

(B17)

Since both the classical action and the volume element are gauge invariant, this is the same as

\[
Z \left[ 0 \right] = \int D\epsilon^{\alpha} \int D\Psi^{i} \text{Det} \left[ \Delta_{\beta}^{\alpha} \left[ \Psi^{i} \right] \right] \delta \left[ f^{\alpha} \left[ \Psi^{i} \right] - c^{\alpha} \right] e^{iS \left[ \Psi^{i} \right]}
\]  

(B18)

This means the group volume may be factored out, thus defining

\[
Z \left[ 0 \right] = \int D\Psi^{i} \text{Det} \left[ \Delta_{\beta}^{\alpha} \left[ \Psi^{i} \right] \right] \delta \left[ f^{\alpha} \left[ \Psi^{i} \right] - c^{\alpha} \right] e^{iS \left[ \Psi^{i} \right]}
\]  

(B19)

In this expression, the correct integration measure is displayed.

It is interesting to check explicitly that this expression is independent of the gauge fixing conditions \( f^{\alpha} \).

Suppose we replace the functions \( f^{\alpha} \) by new gauge fixing conditions \( f^{\alpha} = f^{\alpha} + \delta f^{\alpha} \). At the same time, we change variables in the functional integral to new fields \( \Psi^{i} \) defined by the condition that \( f^{\alpha} \left[ \Psi \right] = f^{\alpha} \left[ \Psi^{i} \right] \).

This change is actually a gauge transform, since we may choose

\[
\Psi^{i} = \Psi^{j} - Q_{j}^{i} \epsilon^{\alpha}
\]  

(B20)

where \( \epsilon^{\alpha} = \left[ \Delta^{-1} \right]_{\beta}^{\alpha} \delta f^{\beta} \). Then the argument of the delta function as well as the exponent remain unchanged. Since the gauge parameters may be field dependent, the volume element is not invariant.
$D\Psi^i = D\Psi^i \text{Det}\frac{\delta\Psi^j}{\delta\Psi^i} = D\Psi^i \left\{1 - (\varepsilon^\gamma Q^\gamma_j)_j\right\}$ \hfill (B21)

Concerning the functional determinant, we have

$$\Delta_{\alpha\beta} = \frac{\delta f^\alpha}{\delta f^\beta} [\Psi] Q^\gamma j [\Psi] = \delta f^\alpha \frac{\delta f^\beta}{\delta f^\alpha} [\Psi] Q^\gamma j [\Psi]$$ \hfill (B22)

$$= f^\alpha Q^\beta - f^\alpha Q^\beta j Q^\gamma j \varepsilon^\gamma + f^\alpha \left[Q^\gamma j \varepsilon^\gamma\right]_j Q^\beta$$ \hfill (B23)

$$= f^\alpha Q^\beta - f^\alpha Q^\beta j Q^\gamma j \varepsilon^\gamma + f^\alpha Q^\gamma j \varepsilon^\gamma Q^\beta + f^\alpha Q^\gamma j \varepsilon^\gamma Q^\beta$$ \hfill (B24)

$$= \Delta_{\alpha\beta} \left[\delta^{\gamma j} + C_{\delta\gamma}^{\alpha\beta} \varepsilon^\delta + \varepsilon^\gamma Q^\beta\right]$$ \hfill (B25)

Since $C_{\delta\gamma}^{\alpha\beta} = 0$,

$$D\Psi^i \text{Det} \left[\Delta_{\alpha\beta} [\Psi^i]\right] = D\Psi^i \text{Det} \left[\Delta_{\alpha\beta} [\Psi^i]\right].$$ \hfill (B26)

This concludes the proof of gauge independence.

Since the persistence amplitude is independent of the $c^\alpha$, we may further average over them with a Gaussian weight $\exp\left[i c^\alpha c^\alpha/2\sigma\right]$. Also the functional determinant may be expressed as a path integral over Grassmann fields

$$\text{Det} \left[\Delta_{\alpha\beta}\right] = \int D\zeta^\alpha D\eta^\beta \exp \left\{-\zeta^\alpha \Delta_{\alpha\beta} \eta^\beta\right\}$$ \hfill (B27)

The final expression looks like an ordinary persistence amplitude for a theory with a modified action functional

$$Z [0] = \int D\Psi^i D\zeta^\alpha D\eta^\beta \exp \left[i S_{FP} \left[\Psi^i, \zeta^\alpha, \eta^\beta\right]\right]$$ \hfill (B28)

$$S_{FP} = S [\Psi^i] + \frac{1}{2\sigma} f^\alpha f^\alpha + i \zeta^\alpha \Delta_{\alpha\beta} \eta^\beta$$ \hfill (B29)

We may use this action to build an effective action in the usual way. If the gauge fixing functions $f$ are chosen conveniently, it is possible to make the effective action gauge invariant as well, thereby becoming the GIEA.

3. The gauge invariant effective action

We now belabor the dependence of the effective action on the gauge fixing functions $f^\alpha$. We have seen that the persistence amplitude is independent of the choice of gauge fixing conditions. Since the effective action reduces to the logarithm of the persistence amplitude when the equations of motion hold (for short, “on shell”), the variation of the effective action with respect to the $f^\alpha$ must be related to the first derivatives of the effective action with respect to the background fields.

To make this explicit, let us consider a change in the gauge fixing condition $f^\alpha \rightarrow f^\alpha + \delta f^\alpha$. As we have seen, the volume element, action, gauge fixing condition and ghost action remain invariant if we simultaneously make a gauge transformation $\Psi^i \rightarrow \Psi^i - Q^\alpha e^\alpha$, where $e^\alpha = \left[\Delta^{-1}\right]_{\beta}^\alpha \delta f^\beta$. But the source terms are not invariant, whereby
\[ \delta \Gamma = \Gamma, \varepsilon \left[ e^{-i\Gamma} \int D\Psi^i D\zeta^\alpha D\eta^\beta Q_i^\alpha e^{i\left[ S_{FP}\left[ \Psi^i, \zeta^\alpha, \eta^\beta \right] - \Gamma, \kappa (\Psi^k - \Phi^k) \right]} \right] \]  

(B30)

This formula is the key to define a gauge invariant effective action. The idea is to allow the gauge fixing conditions \( f^\alpha \) to depend parametrically on the background fields \( \Phi^i \), in such a way that the total variation of the effective action is orthogonal to gauge trajectories

\[ \frac{d\Gamma}{\delta \Phi^i} Q^i_\alpha [\Phi] = \left[ \frac{\delta \Gamma}{\delta \Phi^i} + \frac{\delta \Gamma}{\delta f^\beta} \frac{\delta f^\beta}{\delta \Phi^i} \right] Q^i_\alpha [\Phi] \equiv 0 \]  

(B31)

In view of the previous formula, this means

\[ \Gamma, i Q^j_\alpha [\Phi] e^{-i\Gamma} \int D\Psi^i D\zeta^\alpha D\eta^\beta \left[ \delta^j_\beta + Q^j_\beta [\Psi] \left[ \Delta^{-1} \right]_\beta [\Psi] \frac{\delta f^\beta}{\delta \Phi^j} \right] e^{i\left[ S_{FP}\left[ \Psi^i, \zeta^\alpha, \eta^\beta \right] - \Gamma, \kappa (\Psi^k - \Phi^k) \right]} \equiv 0 \]  

(B32)

Since the \( Q^i_\alpha \) are linear, we may also write

\[ \Gamma, i e^{-i\Gamma} \int D\Psi^i D\zeta^\alpha D\eta^\beta Q^i_\alpha [\Psi] \left[ \Delta^{-1} \right]_\beta [\Psi] \left[ \frac{\delta f^\beta}{\delta \Phi^j} Q^j_\alpha [\Psi] + \frac{\delta f^\beta}{\delta \Phi^j} Q^j_\alpha [\Phi] \right] e^{i\left[ S_{FP}\left[ \Psi^i, \zeta^\alpha, \eta^\beta \right] - \Gamma, \kappa (\Psi^k - \Phi^k) \right]} \equiv 0 \]  

(B33)

The simplest way to satisfy this condition is to choose gauge fixing conditions \( f^\alpha \) invariant under a simultaneous transformation of \( \Phi \) and \( \Psi \) fields, in which case the brackets vanish identically. Observe that since the total derivative of the GIEA is proportional to the partial derivative (that is, with the gauge fixing condition kept fixed), the equations of motion derived from one or the other are equivalent.
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