A Dynamical Self-Consistent Finite Temperature Kinetic Theory:

The ZNG Scheme

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Abstract

We review a self-consistent scheme for modelling trapped weakly-interacting quantum gases at temperatures where the condensate coexists with a significant thermal cloud. This method has been applied to atomic gases by Zaremba, Nikuni, and Griffin, and is often referred to as ZNG. It describes both mean-field-dominated and hydrodynamic regimes, except at very low temperatures or in the regime of large fluctuations. Condensate dynamics are described by a dissipative Gross–Pitaevskii equation (or the corresponding quantum hydrodynamic equation with a source term), while the non-condensate evolution is represented by a quantum Boltzmann equation, which additionally includes collisional processes which transfer atoms between these two subsystems. In the mean-field-dominated regime collisions are treated perturbatively and the full distribution function is needed to describe the thermal cloud, while in the hydrodynamic regime the system is parametrised in terms of a set of local variables. Applications to finite temperature induced damping of collective modes and vortices in the mean-field-dominated regime are presented.

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*This chapter is dedicated to Allan Griffin, an inspirational colleague, mentor and friend who was actively working on these issues until he passed away on 19th May 2011.
I. INTRODUCTION

In most experiments involving Bose–Einstein condensates, the system is only partially condensed, meaning that thermal excitations can play an important role in the damping of condensate collective modes [1–4] or macroscopic excitations such as solitons [5] and vortices [6, 7], making it imperative to include the full dynamics of the non-condensed atoms when modelling such systems. This includes, beyond the usual mean-field contributions, collisions between the non-condensate atoms, and particle-exchanging collisions between the condensate and non-condensate. The approach reviewed in this chapter reflects an accurate representation of these combined dynamics, and can therefore fully simulate the back-action of the thermal cloud on the condensate, which is often neglected, treated to lowest order or in linear response (see Ref. [8]). As this method has been implemented by Zaremba, Nikuni and Griffin (following on from early work by Kirkpatrick and Dorfman [9–12]) we henceforth refer to it as the ZNG method, as described in detail in the recent book of these authors [13].

The strength and frequency of collisions between atoms characterises two distinct dynamical regimes [14]: (i) in the collisionless (or mean-field dominated) regime, in which most experiments with ultracold atomic gases are conducted (in stark contrast to helium), the physics tends to be dominated by mean-field effects; nonetheless, an accurate description of collisions is essential for fully describing the system properties, and accounting for changes in condensate atom number. Importantly, a clear separation of timescales (average collision time is longer that the collective mode period), enables collisions in this regime to be treated perturbatively (see also Ref. [8]). (ii) Some recent experiments have been conducted in the crossover to [2] or deep within the hydrodynamic (or collision dominated) [15] regime. In this regime — which has strong analogies to the two-fluid behaviour of superfluid $^4$He —, the high gas density leads to very rapid collisions between thermal atoms, such that the non-condensate enters a local hydrodynamic equilibrium (a precursor to true thermodynamic equilibrium); this enables its description in terms of a few local hydrodynamic variables (e.g. local density, velocity, chemical potential, temperature, and pressure).

The power of the ZNG theory lies in its ability (i) to successfully describe both collisionless experiments with collective modes [16–18] and macroscopic excitations [19, 20] at finite temperatures (see Section IV); and (ii) to reduce to the damped two-fluid equations of $^4$He in the hydrodynamic limit [21–29] (Section V).
II. METHODOLOGY

The second quantised Hamiltonian for a weakly-interacting Bose gas is given by

$$\hat{H} = \int dr\hat{\Psi}^\dagger(r) \left\{ \left[ -\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(r) \right] + \frac{1}{2} \int dr'\hat{\Psi}^\dagger(r')U(r, r')\hat{\Psi}(r') \right\}\hat{\Psi}(r),$$  \(1\)

where \(V_{\text{ext}}(r)\) is the external confining potential and \(U(r, r') = g\delta(r - r')\) describes binary interactions, with \(g = 4\pi\hbar^2a/m\), where \(a\) is the \(s\)-wave scattering length. Following Beliaev [30], we decompose the second quantised field operator as

$$\hat{\Psi}(r, t) = \phi(r, t) + \hat{\psi}'(r, t),$$  \(2\)

where we define a condensate wavefunction via the non-equilibrium ensemble average \(\phi(r, t) = \langle \hat{\Psi}(r, t) \rangle\), which takes a non-zero value under the assumption of Bose broken symmetry. This in turn implies that \(\langle \hat{\psi}'(r, t) \rangle = 0\), with \(\hat{\psi}'\) capturing all fluctuations around the classical mean-field of the condensate, thus is often termed the non-condensate operator.

By taking an average in the Heisenberg equation of motion for the field operator, \(i\hbar d\hat{\Psi}/dt = [\hat{\Psi}, \hat{H}]\) one obtains the equation of motion for the macroscopic wavefunction (omitting the explicit dependence on \(r\) and \(t\)),

$$i\hbar\frac{\partial\phi}{\partial t} = \left( -\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}} + g\langle \hat{\Psi}^\dagger\hat{\Psi}\rangle \right)\phi + gm'\phi' + g\langle \hat{\psi}'\hat{\psi}' \rangle,$$  \(3\)

which is exact in the context of symmetry-breaking. Expanding the final term using (2), we obtain \(\langle \hat{\Psi}^\dagger\hat{\Psi}\rangle = n_c\phi + m'\phi'^* + 2n'\phi + \langle \hat{\psi}'\hat{\psi}' \rangle\), where we have defined the following mean-field ‘densities’:

- condensate density: \(n_c(r, t) = |\phi(r, t)|^2\),
- non-condensate density: \(n'(r, t) = \langle \hat{\psi}'(r, t)\hat{\psi}'(r, t) \rangle\),
- anomalous pair density: \(m'(r, t) = \langle \hat{\psi}'(r, t)\hat{\psi}'(r, t) \rangle\).

The equation of motion for the condensate therefore reduces to [31–34]

$$i\hbar\frac{\partial\phi}{\partial t} = \left[ -\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}} + g(n_c + 2n') \right]\phi + gm'\phi'^* + g\langle \hat{\psi}'\hat{\psi}' \rangle.$$  \(4\)

Thus the condensate is coupled to higher order correlations which are further coupled to even higher order non-condensate correlations, ad infinitum, suggesting the need for a suitable truncation. An important feature of this equation, highlighted in [31, 33, 34], is that condensate growth from a zero initial value can only arise through the conventionally-neglected ‘anomalous triplet
term $\langle \hat{\psi}'\hat{\psi}'\hat{\psi}' \rangle$, pointing to its importance as a ‘source term’ in condensate kinetics [21]. The corresponding equation of motion for non-condensate atoms reads

$$i\hbar \frac{\partial \hat{\psi}'}{\partial t} = \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}} + 2g(n_c + n') \right] \hat{\psi}' - 2gn'\hat{\psi}' + g\phi^2\hat{\psi}'$$

$$+ g\phi^* (\hat{\psi}'\hat{\psi}' - m') + 2g\phi (\hat{\psi}'\hat{\psi}' - n') + g (\hat{\psi}'^*\hat{\psi}'\hat{\psi}' - \langle \hat{\psi}'^*\hat{\psi}'\hat{\psi}' \rangle).$$

Note that if all the terms $n'(r, t)$, $m'(r, t)$, and $\langle \hat{\psi}'^*\hat{\psi}'\hat{\psi}' \rangle$ are set to zero, Eq. (4) trivially reduces to the zero-temperature Gross–Pitaevskii Equation (GPE). For interacting systems and/or at finite temperatures however, these quantities will in general be present and should be appropriately dealt with.

A. Mean-Field Coupling: First Order Effects

The simplest $T > 0$ Hartree–Fock mean-field method [35–37] is a limiting case of the above equations, in which only normal non-condensate terms involving one creation and one annihilation operator are retained, with anomalous contributions neglected in both Eq. (4) and the entire second line of Eq. (5). In this limit, and upon making a semiclassical approximation for the kinetic energy, the local energy of the thermal atoms becomes in the Hartree–Fock approximation

$$\tilde{\varepsilon}_i(r, t) = \frac{p^2}{2m} + V_{\text{ext}}(r) + 2g[n_c(r, t) + n'(r, t)] \equiv \frac{p^2}{2m} + U_{\text{eff}}(r, t),$$

beyond kinetic energy and external potential, this includes a mean-field potential $U_{\text{eff}}(r, t) = V_{\text{ext}}(r) + 2g[n_c(r, t) + n'(r, t)]$ created by the condensate $n_c(r, t)$ and non-condensate $n'(r, t)$ densities which acts on a thermal atom as it propagates.

In the Hartree–Fock–Bogoliubov (HFB) extension, all quadratic non-condensate operators are maintained in the Hamiltonian, i.e. HFB additionally includes anomalous terms with two like creation or annihilation operators; such an approach, which can also be derived variationally [38], is appealing as it relies on a quadratic Hamiltonian, which can be routinely diagonalised by a Bogoliubov transformation to a quasiparticle basis [36]. Despite explicitly accounting for pair anomalous averages, and providing a lower total energy for the system, this approach is problematic as its homogeneous limit leads to a gap in the energy spectrum at low momenta, which violates the Goldstone theorem [39]. This inconsistency can be avoided by neglecting the anomalous average altogether (or using other tricks [40–44]), as discussed by Griffin [32, 45] and implemented numerically in Refs. [46, 47]. The latter simplified approximation (despite not accounting for...
many-body corrections to the calculations \([40, 45, 48]\) forms a good basis for finite temperature perturbative theories, with higher order effects in \(g\) essential to account for collisional processes.

**B. Particle-Exchanging Collisions: Second Order Effects**

The important collisional processes describing the transfer of an atom into / out of the condensate is contained in the triplet correlation \(\langle \hat{\psi}^+ \hat{\psi}' \hat{\psi}' \rangle\) of Eq. \((4)\) \([21, 31, 34]\). Careful consideration (see also \([33, 49]\)) leads to a dissipative Gross–Pitaevskii equation for the condensate wavefunction \(\phi(\mathbf{r}, t)\) given by \([21]\)

\[
    i\hbar \frac{\partial \phi(\mathbf{r}, t)}{\partial t} = \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) + g \left[n_c(\mathbf{r}, t) + 2n'(\mathbf{r}, t)\right] - iR(\mathbf{r}, t) \right\} \phi(\mathbf{r}, t),
\]

where \(R(\mathbf{r}, t) = -(g/n_c) \text{Im}(\phi^* \langle \psi^* \psi' \psi' \rangle)\), with \(\text{Im}(\ldots)\) denoting the imaginary part, is a non-Hermitian source term which allows the normalisation of the condensate wavefunction \(\phi(\mathbf{r}, t)\) to change with time.

The derivation of the kinetic equation for the non-condensate atoms, based on Eq. \((5)\), follows from the pioneering work of Kirkpatrick and Dorfman \([10, 11]\) on uniform Bose gases as discussed in detail in \([13, 21]\); here we summarise the main results. Key to this is to impose a local semiclassical approximation and to describe the thermal cloud by a distribution function. We thus introduce the Wigner distribution function \(f(\mathbf{p}, \mathbf{r}, t)\) for an atom of momentum \(\mathbf{p}\), at location \(\mathbf{r}\), and time \(t\), defined in terms of the Wigner operator, \(\hat{f}\), for the non-condensate atoms, \(\hat{f}(\mathbf{p}, \mathbf{r}, t) = \int d\mathbf{r}' e^{i\mathbf{p} \cdot \mathbf{r}'/\hbar} \hat{\psi}^+ (\mathbf{r} + \mathbf{r}'/2, t) \hat{\psi}' (\mathbf{r} - \mathbf{r}'/2, t)\). via the expression \(f(\mathbf{p}, \mathbf{r}, t) = \langle \hat{f}(\mathbf{p}, \mathbf{r}, t) \rangle = \text{Tr}[\hat{\rho}(t, t_0) \hat{f}(\mathbf{p}, \mathbf{r}, t)]\); here \(\text{Tr}\) denotes the trace with respect to the density matrix, \(\hat{\rho}(t, t_0)\), whose evolution is defined by \(ih \partial \hat{\rho}(t, t_0)/dt = [\hat{H}_{\text{eff}}(t), \hat{\rho}(t, t_0)]\), where \(\hat{H}_{\text{eff}}(t)\) is an effective Hamiltonian chosen so as to exactly generate the equation of motion for the non-condensate operator of Eq. \((5)\).

It can be split as \(\hat{H}_{\text{eff}}(t) = \hat{H}_{\text{HF}}(t) + \hat{H}'(t)\), where \(\hat{H}_{\text{HF}}(t) = \int d\mathbf{r} \hat{\psi}^+ [-\hbar^2 \nabla^2/2m + U_{\text{eff}}(\mathbf{r}, t)] \hat{\psi}'\) is the unperturbed HF Hamiltonian; the perturbation term \(\hat{H}'(t)\) arises from the difference between contributions of multiples of non-condensate operators and their mean values; see Refs. \([8, 13, 21]\) for more details. The equation of motion for \(f(\mathbf{p}, \mathbf{r}, t)\) thus takes the form

\[
    \frac{\partial f(\mathbf{p}, \mathbf{r}, t)}{\partial t} = \frac{1}{i\hbar} \text{Tr} \left\{ \hat{\rho}(t, t_0) \left[ \hat{f}(\mathbf{p}, \mathbf{r}, t_0), \hat{H}_{\text{eff}}(t) \right] \right\},
\]

\[
    = \frac{1}{i\hbar} \text{Tr} \left\{ \hat{\rho}(t, t_0) \left[ \hat{f}(\mathbf{p}, \mathbf{r}, t_0), \hat{H}_{\text{HF}}(t) \right] \right\} + \frac{1}{i\hbar} \text{Tr} \left\{ \hat{\rho}(t, t_0) \left[ \hat{f}(\mathbf{p}, \mathbf{r}, t_0), \hat{H}'(t) \right] \right\}.
\]
The first term in Eq. (8) [\sim O(g)] generates the usual free-streaming contributions to the Boltzmann equation in the presence of a slowly varying external potential \( U_{\text{eff}}(r, t) \), with a gradient expansion in terms of differentials in position, \( r \) and momentum, \( p \); the second term [\sim O(g^2)] encapsulates the particle evolution due to collisions and gives rise to collisional integrals. We thus obtain the following kinetic Quantum Boltzmann Equation (QBE) (see e.g. [21, 50-52])

\[
\frac{\partial f}{\partial t} + \frac{p}{m} \cdot \nabla_r f - (\nabla_r U_{\text{eff}}) \cdot (\nabla_p f) = C_{12}[f, \phi] + C_{22}[f];
\]

the right hand side of Eq. (9) contains two collisional integrals representing different types of collisions between condensate and non-condensate atoms [9-12]; here thermal excitations are treated semiclassically via Eq. (6).

The collisional integrals involve binary atomic collisions which lead to the scattering of particles from initial to final states, where \( f_i \equiv f(p_i, r, t) \) is the statistical factor for the destruction of a particle in state \( i \) and \((f_i + 1)\), for the stimulated creation of a particle in state \( i \). They are defined as follows:

\[
C_{12}[f, \phi] = \frac{4\pi}{\hbar} g^2|\phi|^2 \int \frac{dp_2}{(2\pi\hbar)^3} \int \frac{dp_3}{(2\pi\hbar)^3} \int \frac{dp_4}{(2\pi\hbar)^3} (2\pi\hbar)^3 \delta(mv_c + p_2 - p_3 - p_4) \\
\times \delta(\epsilon_c + \tilde{\epsilon}_2 - \tilde{\epsilon}_3 - \tilde{\epsilon}_4)(2\pi\hbar)^3 \delta(p - p_2) - \delta(p - p_3) - \delta(p - p_4)) \\
\times [(f_2 + 1)f_3f_4 - f_2(f_3 + 1)(f_4 + 1)],
\]

refers to a collision involving one condensate atom with one non-condensate atom and results in atom transfer between the two subsystems, and

\[
C_{22}[f] = \frac{4\pi}{\hbar} g^2 \int \frac{dp_2}{(2\pi\hbar)^3} \int \frac{dp_3}{(2\pi\hbar)^3} \int \frac{dp_4}{(2\pi\hbar)^3} (2\pi\hbar)^3 \delta(p + p_2 - p_3 - p_4) \\
\times \delta(\epsilon + \tilde{\epsilon}_2 - \tilde{\epsilon}_3 - \tilde{\epsilon}_4)(f + 1)(f_2 + 1)f_3f_4 - f_2(f_3 + 1)(f_4 + 1)]
\]

refers to a collision involving the redistribution of two non-condensate atoms.

In the absence of the collisional terms \( C_{12} \) and \( C_{22} \) in Eq. (9), the equation is known as the Vlasov equation, arising in diverse fields of physics such as plasma physics, condensed matter physics and astrophysics. \( C_{22} \) is the usual collisional term appearing in the ordinary bosonic Boltzmann equation (in the absence of condensation). Setting \( C_{22}[f] = 0 \), as appropriate in thermodynamic equilibrium, implies that particles are distributed according to the Bose–Einstein distribution \( f_i \to n_{\text{BE}}(\tilde{\epsilon}_i) = [e^{\tilde{\epsilon}_i/kT} - 1]^{-1} \). In the presence of a condensate, \( C_{12} = 0 \) when the condensed and non-condensate subsystems are in local ‘diffusive’ equilibrium, implying that there is
no net transfer of particles between the two subsystems on average. In cases out of equilibrium, this term acts to transfer atoms between the condensed and non-condensed parts of the system, with overall particle number conservation ensured by the source term in Eq. (7) being given by,

\[ R(r, t) = \frac{\hbar}{2|\phi(r, t)|^2} \int \frac{dp}{(2\pi\hbar)^3} C_{12}[f(p, r, t), \phi(r, t)]. \] (12)

The delta functions of Eqs. (10) and (11), enforce conservation of energy and momentum; condensate atoms appearing in \( C_{12} \) have energy \( \varepsilon_c = m v_c^2 / 2 + \mu_c \), and momentum \( m v_c \), where \( \mu_c \) is the condensate chemical potential. Although the exact expression for \( \mu_c \) depends on pair and triplet anomalous averages [21], within ZNG their static values are not included in \( \mu_c \) or in the excitation energies (which are both treated to first order in \( g \)), thus yielding the reduced expression

\[ \mu_c(r, t) = -\frac{\hbar^2 \nabla^2 \sqrt{n_c(r, t)}}{2m \sqrt{n_c(r, t)}} + V_{\text{ext}}(r) + gn_c(r, t) + 2gn'(r, t). \] (13)

It is crucial to note that this does not imply that the simultaneous annihilation or creation of more than one particle are ignored, since such terms are implicitly maintained (in an approximate, yet consistent manner) to second order in \( g \) in the dynamical equations, thus giving rise to the collisional integral \( C_{12} \). While this procedure is approximate, the method used here is internally self-consistent, and eventually leads to a theory which conserves both total energy and total particle number.

To make contact with physical variables, we note that the non-condensate density can be reconstructed from the distribution function via

\[ n'(r, t) = \int \frac{dp}{(2\pi\hbar)^3} f(p, r, t). \] (14)

Equations (7) and (9) are the closed set of ZNG equations for a condensate coexisting in a trap with a cloud of thermal excitations. Their solution governs the evolution of the physical variables of interest.

C. Numerical Implementation

Equation (7) is solved in much the same way as the simpler, \( T = 0 \) GPE, with the non-condensate mean field and the source term calculated from the QBE at each time step; we briefly outline the numerical procedure for solving the QBE (9) in the mean-field-dominated regime, where the full distribution function \( f(p, r, t) \) is required to accurately describe the thermal cloud — see [53] for details.
We simulate the evolution of the thermal cloud phase space distribution by means of a set of test particles. This allows a Lagrangian approach to be adopted, whereby the motion of a phase point is followed in time according to Newton’s equations of motion $d\mathbf{r}_i(t)/dt = \mathbf{p}_i(t)/m$ and $d\mathbf{p}_i(t)/dt = -\nabla U_{\text{eff}}(\mathbf{r}, t)$. These are initially distributed in phase space according to $f(\mathbf{p}, \mathbf{r}, t) \approx \gamma (2\pi \hbar)^3 \sum_{i=1}^{N_{tp}} \delta(\mathbf{r} - \mathbf{r}_i(t)) \delta(\mathbf{p} - \mathbf{p}_i(t))$, where $\gamma = N'/N_{tp}$ is a weighting factor which ensures that the physical number $N'$ of thermal atoms is being represented. As test particles are only used in order to accurately sample the distribution, there is no need for their number to match the actual number of thermal atoms, which can be smaller or larger, with the only requirement that $N_{tp}$ needs to be sufficiently large to minimise the effects of using a discrete particle description.

The density at a particular grid point can be determined by using a cloud-in-cell method [54]. This method takes into account the actual position of a particle within a cell, and also allows for migrations between grid cells. As residual fluctuations remain, additional smoothing is necessary, achieved through convolving the densities with a Gaussian of width a few times the thermal cloud grid spacing (the condensate density is also convolved for consistency except in simulations involving solitons and vortices, where the main physical effects would become smeared out). At the end of each time step, the probability that a given test particle suffers a collision is determined and its position and velocity are updated accordingly (respecting momentum and energy conservation). The collisions are treated using a Monte Carlo sampling technique: whether a collision has occurred, and what its type is, is determined by comparison of the calculated collisional probability with a random number. Finally, the condensate evolution is appropriately amended by the occurrence of any collisions which transfer particles into/out of the condensate. As collisions are dealt with separately from the dynamical evolution, we are able to choose which collisional effects to include in our simulations, and thus assess the importance of each contribution in a physical setting, thereby enabling a comparison to other theories (in appropriate limits).

D. ZNG Condensate Hydrodynamics

Introducing phase and amplitude variables to the condensate wavefunction $\phi(\mathbf{r}, t) = \sqrt{n_c(\mathbf{r}, t)} e^{i \theta(\mathbf{r}, t)}$ allows Eq. (4) to be recast in hydrodynamic form:

$$\frac{\partial n_c}{\partial t} = \nabla \cdot (n_c \mathbf{v}_c) = -\Gamma_{12} [f, \phi]$$

and

$$m \frac{\partial \mathbf{v}_c}{\partial t} = -\nabla \left( \mu_c + \frac{1}{2} m \mathbf{v}_c^2 \right).$$

(15)
The condensate velocity is given by \( \mathbf{v}_c(\mathbf{r}, t) \equiv (\hbar/m)\nabla\theta(\mathbf{r}, t) \), \( \mu_c \) is defined by Eq. (13) and \( \Gamma_{12}[f, \phi] \equiv \Gamma_{12}(\mathbf{r}, t) = 2n_c R(\mathbf{r}, t)/\hbar \) is the ‘source’ term due to particle-exchanging collisions between condensate and thermal cloud.

### III. VALIDITY ISSUES

#### A. Validity Domain

A key feature of a successful theory for describing bosonic quantum fluids is its ability to explain the phenomenon of superfluidity. This arises naturally within ZNG, since the condensate velocity \( \mathbf{v}_c \) is precisely the velocity describing the flow of the superfluid density in the two-fluid model. Although the ZNG equations are based on the Beliaev scenario, this is done here within certain approximations for the excitations, namely that they are single-particle-like (Hartree–Fock) and they ignore anomalous averages. Thus, the present implementation is inappropriate for describing collective phonon-like excitations which become important at very low temperatures. This could nonetheless be remedied, in favour of Bogoliubov quasiparticles, since the nature of the excitation spectrum is intrinsic to the choice of the Hamiltonian on which perturbation theory is applied; hence the formalism presented here could also be systematically extended within the Beliaev field-theoretic approach to account for such features (see Appendix A of Ref. [21], Chapters 3 and 17 of Ref. [13] and Ref. [8]).

The ZNG theory has been remarkably successful in describing a range of dynamical problems, across an extremely broad temperature range, in both the collisionless and hydrodynamic regimes; it even describes the rather involved problem of condensate growth [55], provided an initial ‘seed’ condensate is assumed. However, its present implementation will fail in the regime of critical fluctuations, i.e. very close to the transition temperature in 3d systems, or over broader temperature ranges in 1d/2d systems which exhibit enhanced phase fluctuations.

#### B. Relevance to Other Theories

The ZNG theory is formally related to the approach of Walser et al. [56, 57], Köhler et al. [58] and Proukakis et al. [31, 34, 49], which amounts to a similar perturbative treatment starting however from an appropriately generalised basis which includes the pair anomalous average. However, an important advantage of ZNG is its formulation in terms of phase space distribution functions,
which allows for a relatively straightforward numerical implementation, that can be extended to the hydrodynamic regime. (The closely-related explicitly number-conserving approach \cite{59,61} has not yet been formulated in terms of a self-consistently evolving thermal cloud.)

This book also describes a number of stochastic classical-field approaches (see e.g. \cite{62–65}). In some sense, the ZNG theory can be thought of as the analogue of the full theory of Stoof \cite{62}, when derived within a symmetry-breaking perspective. The key difference of the ZNG formulation compared to those of classical field methods is that the ZNG approach directly describes the condensate order parameter, whereas the field appearing in the GPE-like equation of classical field theories describes a range of ‘classical’ or ‘coherent’ modes which include, but are not restricted to, the condensate mode. In such theories, the latter is to be extracted (in the Penrose–Onsager sense) by numerical diagonalisation \textit{a posteriori}. In contrast to this, the ZNG method \textit{directly} generates two distinct components, the condensate and the non-condensate (see Fig. 2), and thus it provides an intuitive picture of the fundamental physical processes taking place in a partially-condensed system; this also guarantees a direct link to the superfluid properties of the system — which are harder to extract from unified stochastic approaches — thus leading directly to established theories of superfluid helium (see Section V). On the implementation front, the current importance of ZNG is that it includes a fully dynamical thermal cloud self-consistently; this is crucial, e.g. in order to correctly predict the Kohn mode induced when suddenly displacing the trap, whereas stochastic methods describing a band of modes coupled to a static thermal cloud would actually lead to artificial damping.

IV. APPLICATIONS

A. Damping of Condensate Scissors Mode

By analogy with earlier work in nuclear physics (see \cite{66} for a review), the superfluid nature of a BEC can be probed by observing the so-called ‘scissors mode’; this can be excited \cite{67} by adiabatically rotating an axially symmetric trapping potential of the form

\[
V_{\text{ext}}(\mathbf{r}) = \frac{m(\omega_\rho^2 \rho^2 + \omega_z^2 z^2)}{2},
\]

through a small angle \(\theta_0\) about the \(y\)-axis, and then suddenly in the opposite direction through an angle \(-2\theta_0\). The observation of a single frequency signals the irrotational flow of the condensate. This should be contrasted to the superposition of two frequencies for the thermal component, whose flow has both rotational and irrotational character. Simulations with the ZNG theory by
Jackson and Zaremba [17] found excellent agreement for $T < 0.8T_C^0$ with a subsequent experiment [8] measuring the temperature dependence of the frequency and damping of such oscillations. The inclusion of collisional processes associated with both $C_{12}$ and $C_{22}$ is crucial for explaining the experimental observations, and simulations performed without collisions result in up to 50% lower damping rates. The Landau damping process is thus a product of both collisional and mean-field effects.

FIG. 1: (a) Frequency and (b) damping rate of the scissors mode for a variable total number of atoms, intended to simulate the experiment of Ref. [3]. The condensate mode is indicated by open (theory) and filled (experiment) circles. The open squares in (b) show the calculated average damping rate of the two thermal cloud modes, while the filled squares are the corresponding experimental values. Reprinted with permission from B. Jackson and E. Zaremba, *Finite-temperature simulations of the scissors mode in Bose–Einstein condensed gases*, Phys. Rev. Lett. 87, 100404 (2001) [17]. Copyright (2001) by the American Physical Society.
B. Decaying Vortex Dynamics

The thermal cloud leads to dissipation of an off-centred vortex at finite temperatures, causing it to minimise its energy in a harmonically-trapped condensate by moving out of the condensate radially [6, 7]. Figure 2 (right) shows the nonlinear increase of the decay rate with increasing temperature, clearly highlighting the role of all collisional processes, particularly at higher temperatures [20]. The largest increase in damping rates arises from the particle-exchanging $C_{12}$ collisions. Our results are compared to the analytic predictions of Fedichev and Shlyapnikov [68] (FS), which account for the scattering of thermal excitations from the vortex core, and those of

![Image](image_url)

**FIG. 2:** Left: Density cross sections of the condensate (top) and thermal cloud (bottom) ($T = 0.5T_C$) showing clearly the two distinct components simulated within ZNG. Colours range from black (low density) to white (high density) with different scales for the two images. Right: (Inset) Log-linear plot of vortex radial position as a function of time for $T = 0.7T_C$ (solid line); the dashed line is an exponential fit, $r_v(t) = r_0 e^{\gamma t}$, to the data over $0 \leq \omega \perp t \leq 50$. (Main Plot) Values of $\gamma$ based on different levels of approximation: static thermal cloud with condensate dissipation, $iR$, included (solid circles), thermal cloud allowed to evolve within the QBE (Eq. (9)) without collisions (open circles), with only thermal-thermal collisions (pluses), with only particle-transferring collisions (stars) or with all collisional processes (squares). For comparison, analytic predictions of FS [68] (solid line) and DLS [69] (dashed line) are shown. (Calculations performed at fixed condensate number, $N_c \approx 10,000$, and an initial radial vortex offset $r_0 = 0.26R_{TF}$ from the trap centre).
Duine, Leurs, and Stoof \cite{69} (DLS), which include the effects of $C_{12}$ collisions within the static thermal cloud approximation; the latter are in full agreement with our results, in the corresponding limit of condensate dissipation from a static thermal cloud. The enhanced decay predicted by the full theory highlights the importance of including all dynamical processes in modelling experiments. (See also Ref. \cite{19} for the corresponding dark soliton analysis accurately reproducing the experiment \cite{5}.)

V. RELEVANCE TO OTHER SYSTEMS

By construction, based on its symmetry-breaking formulation, the ZNG approach is consistent with prevailing theories for the description of superfluid helium (see also Ref. \cite{13}). In the hydrodynamic (or collision-dominated) regime, when the thermal cloud enters a state of local hydrodynamic equilibrium, Landau’s famous 2-fluid equations for the superfluid and normal densities arise as a special case of the ZNG equations \cite{13, 21, 22}, when the condensate and thermal cloud are in diffusive local equilibrium with the same chemical potential. These equations can be extended to include hydrodynamic damping, which arises when the distribution functions deviates from its local equilibrium form, giving rise to the Landau–Khalatnikov two-fluid hydrodynamic equations \cite{23}, of liquid helium, with the correct transport coefficients, thus facilitating a precise determination of the crossover between the mean-field collisionless and two-fluid hydrodynamic regime. It would be of interest to extend the ZNG formalism to other situations such as dipolar Bose gases, spinor condensates, bosonic mixtures and apply this scheme to trapped superfluid Fermi gases.

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[1] D. S. Jin, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 78, 764 (1997).
[2] D. M. Stamper-Kurn, H.-J. Miesner, S. Inouye, M. R. Andrews, and W. Ketterle, Phys. Rev. Lett. 81, 500 (1998).
[3] O. Maragò, G. Hechenblaikner, E. Hodby, and C. Foot, Phys. Rev. Lett. 86, 3938 (2001).
[4] F. Chevy, V. Bretin, P. Rosenbusch, K. W. Madison, and J. Dalibard, Phys. Rev. Lett. 88, 250402 (2002).
[5] S. Burger, K. Bongs, S. Dettmer, W. Ertmer, K. Sengstock, A. Sanpera, G. V. Shlyapnikov, and M. Lewenstein, Phys. Rev. Lett. 83, 5198 (1999).
[6] P. Rosenbusch, V. Bretin, and J. Dalibard, Phys. Rev. Lett. 89, 200403 (2002).
[7] J. R. Abo-Shaeer, C. Raman, and W. Ketterle, Phys. Rev. Lett. 88, 070409 (2002).
[8] N. P. Proukakis and B. Jackson, Journal of Physics B: Atomic, Molecular and Optical Physics 41, 203002 (2008).
[9] T. R. Kirkpatrick and J. R. Dorfman, Phys. Rev. A 28, 2576 (1983).
[10] T. R. Kirkpatrick and J. R. Dorfman, Journal of Low Temperature Physics 58, 399 (1985).
[11] T. R. Kirkpatrick and J. R. Dorfman, Journal of Low Temperature Physics 58, 301 (1985).
[12] T. R. Kirkpatrick and J. R. Dorfman, Journal of Low Temperature Physics 59, 1 (1985).
[13] A. Griffin, T. Nikuni, and E. Zaremba, Bose-condensed gases at finite temperatures (Cambridge University Press, 2009).
[14] A. Griffin, Excitations in a Bose-condensed liquid, Cambridge studies in low temperature physics (Cambridge University Press, 1993).
[15] R. Meppelink, S. B. Koller, J. M. Vogels, H. T. C. Stoof, and P. van der Straten, Phys. Rev. Lett. 103, 265301 (2009).
[16] J. E. Williams and A. Griffin, Phys. Rev. A 63, 023612 (2001).
[17] B. Jackson and E. Zaremba, Phys. Rev. Lett. 87, 100404 (2001).
[18] B. Jackson and E. Zaremba, Laser Phys. 12, 93 (2002).
[19] B. Jackson, N. P. Proukakis, and C. F. Barenghi, Phys. Rev. A 75, 051601 (2007).
[20] B. Jackson, N. P. Proukakis, C. F. Barenghi, and E. Zaremba, Phys. Rev. A 79, 053615 (2009).
[21] E. Zaremba, T. Nikuni, and A. Griffin, Journal of Low Temperature Physics 116, 277 (1999).
[22] T. Nikuni, E. Zaremba, and A. Griffin, Phys. Rev. Lett. 83, 10 (1999).
[23] T. Nikuni and A. Griffin, Phys. Rev. A 63, 033608 (2001).
[24] T. Nikuni and A. Griffin, Phys. Rev. A 65, 011601 (2001).
[25] T. Nikuni and A. Griffin, Journal of Low Temperature Physics 111, 793 (1998).
[26] T. Nikuni, Phys. Rev. A 65, 033611 (2002).
[27] A. Griffin and E. Zaremba, Phys. Rev. A 56, 4839 (1997).
[28] T. Nikuni and A. Griffin, Phys. Rev. A 69, 023604 (2004).
[29] E. Zaremba, A. Griffin, and T. Nikuni, Phys. Rev. A 57, 4695 (1998).
[30] S. T. Beliaev, Sov. Phys. JETP 7, 289 (1958).
[31] N. P. Proukakis and K. Burnett, J. Res. Natl. Inst. Stand. Technol. 101, 457 (1996).
[32] A. Griffin, Phys. Rev. B 53, 9341 (1996).
[33] N. P. Proukakis, Ph.D. thesis, University of Oxford (1997).
[34] N. P. Proukakis, K. Burnett, and H. T. C. Stoof, Phys. Rev. A 57, 1230 (1998).
[35] S. Giorgini, L. Pitaevskii, and S. Stringari, Journal of Low Temperature Physics 109, 309 (1997).
[36] C. Pethick and H. Smith, Bose-Einstein condensation in dilute gases (Cambridge University Press, 2002).
[37] L. P. Pitaevskii and S. Stringari, Bose-Einstein Condensation (Oxford University Press, Great Clarendon Street, Oxford, 2003).
[38] J. Blaizot and G. Ripka, Quantum theory of finite systems (MIT Press, 1986).
[39] J. Binney, The Theory of critical phenomena: an introduction to the renormalization group, Oxford science publications (Clarendon Press, 1992).
[40] M. Bijlsma and H. T. C. Stoof, Phys. Rev. A 55, 498 (1997).
[41] N. P. Proukakis, S. A. Morgan, S. Choi, and K. Burnett, Phys. Rev. A 58, 2435 (1998).
[42] V. I. Yukalov and H. Kleinert, Phys. Rev. A 73, 063612 (2006).
[43] P. Tommasini, E. J. V. de Passos, M. O. C. Pires, and A. F. R. de Toledo Piza, Journal of Physics: Condensed Matter 17, 3165 (2005).
[44] T. Kita, J. Phys. Soc. Japan 75, 044603 (2006).
[45] H. Shi and A. Griffin, Physics Reports 304, 1 (1998).
[46] D. A. W. Hutchinson, E. Zaremba, and A. Griffin, Phys. Rev. Lett. 78, 1842 (1997).
[47] D. A. W. Hutchinson, K. Burnett, R. J. Dodd, S. A. Morgan, M. Rusch, E. Zaremba, N. P. Proukakis,
M. Edwards, and C. Clark, Journal of Physics B: Atomic, Molecular and Optical Physics 33, 3825 (2000).

[48] K. Burnett, in Bose-Einstein Condensation in Atomic Gases (Proc. Int. School of Physics Enriko Fermi, Italian Physical Society, 1999), p. 265.

[49] N. P. Proukakis, Journal of Physics B: Atomic, Molecular and Optical Physics 34, 4737 (2001).

[50] D. Jaksch, C. W. Gardiner, and P. Zoller, Phys. Rev. A 56, 575 (1997).

[51] O. J. Luiten, M. W. Reynolds, and J. T. M. Walraven, Phys. Rev. A 53, 381 (1996).

[52] M. Holland, J. Williams, and J. Cooper, Phys. Rev. A 55, 3670 (1997).

[53] B. Jackson and E. Zaremba, Phys. Rev. A 66, 033606 (2002).

[54] R. W. Hockney and J. W. Eastwood, Computer simulation using particles (Taylor & Francis, Inc., Bristol, PA, USA, 1988).

[55] M. J. Bijlsma, E. Zaremba, and H. T. C. Stoof, Phys. Rev. A 62, 063609 (2000).

[56] R. Walser, J. Williams, J. Cooper, and M. Holland, Phys. Rev. A 59, 3878 (1999).

[57] R. Walser, J. Cooper, and M. Holland, Phys. Rev. A 63, 013607 (2000).

[58] T. Köhler and K. Burnett, Phys. Rev. A 65, 033601 (2002).

[59] C. W. Gardiner, Phys. Rev. A 56, 1414 (1997).

[60] S. A. Gardiner and S. A. Morgan, Phys. Rev. A 75, 043621 (2007).

[61] Y. Castin and R. Dum, Phys. Rev. A 57, 3008 (1998).

[62] H. T. C. Stoof, Journal of Low Temperature Physics 114, 11 (1999).

[63] P. Blakie, A. Bradley, M. Davis, R. Ballagh, and C. Gardiner, Advances in Physics 57, 363 (2008).

[64] C. Lobo, A. Sinatra, and Y. Castin, Phys. Rev. Lett. 92, 020403 (2004).

[65] M. Brewczyk, M. Gajda, and K. Rzazewski, Journal of Physics B: Atomic, Molecular and Optical Physics 40, R1 (2007).

[66] N. L. Iudice, Physics of Particles and Nuclei 28, 556 (1997).

[67] O. M. Maragò, S. A. Hopkins, J. Arlt, E. Hodby, G. Hechenblaikner, and C. J. Foot, Phys. Rev. Lett. 84, 2056 (2000).

[68] P. O. Fedichev and G. V. Shlyapnikov, Phys. Rev. A 60, R1779 (1999).

[69] R. A. Duine, B. W. A. Leurs, and H. T. C. Stoof, Phys. Rev. A 69, 053623 (2004).