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QUANTUM KINETIC THEORY FOR A BOSE-EINSTEIN CONDENSED ALKALI GAS

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The most salient features of the Bose-Einstein condensation of a magnetically confined alkali vapor is the diluteness of the gas and the extremely weak effective interactions. From a theoretical point of view, the interesting aspect is the potential formulation of the many-body quantum theory for a non-uniform and potentially non-equilibrium system founded entirely on microscopic physics. The crucial postulate is the rapid attenuation of many particle quantum correlations in the dilute system which can be motivated from universal considerations. In principle, it will be possible to provide direct comparison between theory and experiment over all temperature scales with no phenomenological parameters—a challenge facing the theoretical community in the near future. The dilute gas experiments provide an exciting stage on which to build bridges linking the theory of complex and collective phenomena in superconducting and superfluid systems, with the single particle microscopic physics described in quantum optics and laser physics.

1 Development of a kinetic theory

Since the recent demonstration of Bose-Einstein condensation in 1995 in experiments probing the physics of ultracold gases,[1] there has been renewed theoretical activity investigating many novel properties of confined and weakly-interacting condensates. A major area of focus has been zero temperature theory where the time-dependent Gross-Pitaevskii equation describes the evolution of the macroscopic wave function for the condensate. There is already a tremendously rich literature on the predictions of this equation for a variety of experimental situations—often with strong agreement with experimental observation.[2]

From a broader perspective, a more fundamental problem is the description of the non-zero temperature regime where one must consider systematically the interactions between the condensate and the non-condensate components. Recent work has considered this problem within the Hartree-Fock-Popov approximation (HFP).[3] This approximation considers the dynamic evolution of the condensate in much the same way as in the Gross-Pitaevskii equation, but includes the effects of the self-consistent potential arising from the mutual interaction between the condensate and non-condensate components. However, the non-condensate atoms are treated in a completely static manner and the equilibrium form of the distribution function of the populations is assumed. Improvements of this theoretical framework can be made to include the effects of fluctuations in the density of the non-condensate component with the usual random phase approximation (RPA).[4]

These approaches attempt to describe the collective system in the collisionless mean-field regime but do not encapsulate all the essential physics. They do not account for population transfer between the condensate and non-condensate degrees of freedom, nor do they incorporate the off-diagonal self-energy terms (the anomalous densities) believed to be important at low temperature. While they provide a

first step, many of the binary collisional diagrams are omitted in these simple theories, essentially without justification. These diagrams must be included in order to develop a quantitative theory for comparison with experiment. The principal difficulty is the lack of a relevant local equilibrium approximation and the breaking of translational invariance due to the presence of the trapping potential. Instead the calculated mean-free path between collisions is typically longer than the size of the system. One is therefore not able to use directly many of the well-established techniques which are applicable to the uniform gas, and instead new theoretical methods are required to treat aspects specific to this problem.

Our approach is based on a derivation of the quantum kinetic theory from first principles as described in detail in Walser *et al.*[5] The required elements are founded on the formative historical work of Gilbert, Chapman, and Enscog[6] who showed that even for complex systems, an appropriate abbreviated description may be derived from which all relevant observables can be obtained. This approach was extended to the quantum gas by Bogoliubov and von Neumann who developed the use of a course-grained statistical operator for quantum Markovian systems. Recent derivations of quantum kinetic theory founded on similar physical ideas are given in Akheizer and Peletminskii,[7] Kane and Kadanoff,[8] Kirkpatrick and Dorfmann,[9] Zubarev, Morozov, and Röpke,[10] and Blaizot and Ripka.[11]

Based on such a microscopic picture of the weakly interacting bosonic gas, we derive a generalized kinetic theory for a Markovian many-body density operator. The density operator is functionally dependent on a few key variables which must be carefully chosen as we will discuss. These quantities serve as master variables and determine the system's evolution on a coarse-grained time scale. The weak interactions allow a perturbative expansion of the evolution, from which we obtain kinetic equations that describe the dynamics of the expectation value of any single-time observable.

There are also other approaches to finite temperature quantum theory for the dilute Bose and Fermi gases which have been motivated by the recent alkali experiments. In addition to the mean-field description mentioned previously (HFP and RPA) there are direct attempts to solve the many-particle Schrödinger equation,[12] application of renormalization techniques,[13] alternative derivation of a quantum kinetic master equation,[14] and formulation of the non-zero temperature theory in the hydrodynamic limit.[15] One of the difficulties has been connecting these different methods and establishing that the approaches are isomorphic since they are formulated to describe the same physical system. This difficulty arises principally from the fact that the set of physical assumptions which are made are not necessarily all equivalent. The quantum theory we present here is founded on an appropriate set of assumptions for the dilute alkali gas which can be extremely well motivated. In order to highlight this key point, we now address each of the key assumptions individually.

1.1 Separation of time scales

The motion of trapped atoms in a dilute gas consists of free oscillations within the external potential that are interrupted by short binary collision events (see Fig. 1).

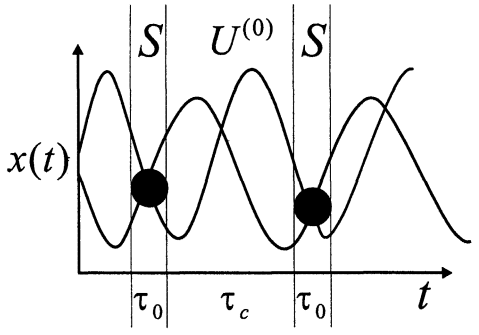

Figure 1. One dimensional illustration of particle trajectories in a harmonic potential. The long periods of free oscillations are interrupted by short collision events in which the particles are strongly correlated.

The range of the two-particle potential characterizing the collisions is given by the scattering length a_s. The duration of a collision event is characteristically the ratio of the scattering length to the average velocity v of a particle in the gas, i.e. $\tau_0 = a_s/v$. This time scale is extremely short, typically in the microsecond to nanosecond range even for the ultracold gases. The other important time scale is the inverse collision rate $\tau_c = (na_s^2 v)^{-1}$ where n is the number density of atoms (we ignore geometrical factors such as the 8π in the collisional cross-section for the purposes of these scaling arguments). The time τ_c is typically on the order of one second. This implies a separation of time scales given by

$$\tau_c \gg \tau_0$$

which can be rearranged to give the diluteness criterion of the gas

$$na_s^3 \ll 1.$$

The time scale separation implies the existence of a kinetic stage preceding equilibrium. Such a kinetic stage is absent in strongly interacting systems where a local equilibrium is established immediately and where the hydrodynamic theory ($\tau_c \approx \tau_0$) is applicable.

1.2 Markov approximation

Each individual collision quantum mechanically entangles the states of the participating atoms. However, since the gas is dilute, prior to the same atoms interacting again, they will collide with other atoms from the gas ensemble, and memory of the original collision event will be erased. This principle is a statement of the rapid attenuation of multiparticle quantum correlations and is founded on very universal considerations. It is required to introduce irreversibility into the quantum theory associated with relaxation towards equilibrium. The memory erasure implies that the evolution of the system is determined only by its present state—a situation familiar whenever a Markov approximation is applicable. The attenuation of correlations principle motivates the existence of key variables which determine the

evolution. This is due to the fact that the information required to specify the many-body quantum state is greatly reduced if limits are placed on the role of many-body quantum correlations. Determining these key variables is a crucial element of the theoretical formulation.

1.3 Course grained density operator

We course-grain the time evolution by averaging over the τ_0 time scale to avoid tracking the complicated (and irrelevant) dynamics which describe the motion of two atoms during a collision. We are interested here only in the evolution on the relaxation time scale determined by τ_c. Within the Markov approximation, the evolution of the exact many-body density operator $\rho(t)$ is given by the course-grained statistical density operator σ which has no intrinsic time dependence, but depends functionally on a set of dynamic master variables $\{\gamma_i(t)\}$, i.e.

$$\rho(t) \approx \sigma_{\{\gamma_i(t)\}}.$$

The interactions are sufficiently weak that one may develop a perturbation theory by expanding the evolution in powers of the small parameter a_s (in this expansion the effect of the mean-field must be accounted for carefully.) Truncating this cluster expansion at first order is sufficient for the dilute gas.

1.4 Single particle basis

The theory can be formulated in any complete single particle basis. This will typically include quantum numbers for both internal states of the atom, such as the hyperfine level F and Zeeman state m_F, as well as external spatial quantum numbers determined by the form of the confining potential. For the tightly confined interacting gas, plane wave solutions are not usually appropriate, nor are the quantum numbers for the three-dimensional harmonic trap n_x, n_y, n_z, since they do not account for the effect of the mean-field. An appropriate choice is the eigenmodes of the potential seen by the non-condensate component as illustrated in Fig. 2.

Although any complete basis may be used, a careful choice will result in a simplified description of the dynamics.

1.5 Master variables

The master variables for the dilute gas include all single and quadratic operator terms, i.e.

- $\hat{a}_1$, $\hat{a}_2^\dagger$
- $\hat{f}_{12} = (\hat{a}_2^\dagger - \alpha_2^*)(\hat{a}_1 - \alpha_1)$,
- $\hat{m}_{12} = (\hat{a}_2 - \alpha_2)(\hat{a}_1 - \alpha_1)$,
- $\hat{n}_{12} = (\hat{a}_2^\dagger - \alpha_2^*)(\hat{a}_1^\dagger - \alpha_1^*)$,

where $\hat{a}_1$ annihilates an atom in single particle state $|1\rangle$ and has an expectation value of $\alpha_1 = \langle \hat{a}_1 \rangle$.

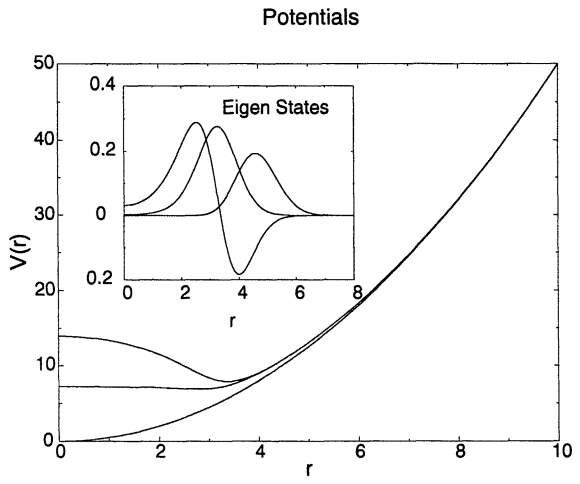

Figure 2. Potentials for the isotropic harmonic oscillator of angular frequency $\omega = 2\pi \times 200$ Hz for 10000 ^{87}Rb atoms. In order of increasing energy, the potentials are: the trapping potential, the potential seen by the condensate, and the potential seen by the non-condensate. Example eigenstates of the non-condensate potential are given in the inset. Natural harmonic oscillator units are used: $\hbar\omega$ for energy, and $(\hbar/m\omega)^{1/2}$ for length, where m is the atomic mass.

We are motivated to choose this set by the known form of the theory in the low and high temperature limits. At high temperature, we wish to recover classical kinetic theory as given by the Boltzmann transport equation, where the description in terms of populations, $\tilde{f}_{11} = \langle \hat{f}_{11} \rangle$, is complete. As the temperature is decreased below the critical temperature for Bose-Einstein condensation, it is necessary to increase the set of master variables to include off-diagonal coherences, $\tilde{f}_{12} = \langle \hat{f}_{12} \rangle$, $\tilde{m}_{12} = \langle \hat{m}_{12} \rangle$ and $\tilde{n}_{12} = \langle \hat{n}_{12} \rangle$, and the presence of the mean field, α_1. At zero temperature, we recover the Gross-Pitaevskii theory including the effects of depletion of the condensate.

An important point is that this is the most general set containing mean values of pairs of operators. The Gaussian form for the many-body density operator which is implicitly assumed is

$$\sigma_{\{\gamma_i\}} = \exp\left(\Omega - \hat{f}_{12}\Upsilon^{12} - \hat{m}_{12}\Lambda^{12} - \hat{n}_{12}\Lambda^{12*}\right)$$

where Ω is the free energy, and Υ and Λ are the conjugate variables (complex numbers) associated with each of the master variables (operators). Note that we always use the convention that repeated indices imply summation. Maintaining this Gaussian form is necessary in order to express higher moments in terms of first and second moments through the repeated use of Wick's theorem.[11] Therefore, if one attempts to derive a more general theory by explicitly including operator triples or higher order terms, the solution is typically intractable. An important feature of the Gaussian form is that it automatically insures positive definiteness, so that all populations of single particle states are greater than zero.

2 Kinetic master equations

Within the limits of the Born-Markov approximations, we have derived a complete second-order kinetic theory. By applying Wick's theorem methodically, we were able to obtain self-consistent equations for the mean field $\alpha = \alpha_1 \, |1\rangle$ (summation is implied), and to generalize the quantum Boltzmann equation to normal fluctuations $\tilde{f} = \tilde{f}_{12} \, |1\rangle \langle 2|$, anomalous fluctuations $\tilde{m} = \tilde{m}_{12} \, |1\rangle |2\rangle$, and the adjoint anomalous fluctuations $\tilde{n} = \tilde{n}_{12} \, \langle 1| \langle 2|$.

2.1 Mean-field equations

The kinetic mean-field equations describe the motion of the condensed fraction immersed in a cloud of non-condensate atoms. By discarding all of the interactions, except the condensate's self-interaction, these equations reduce to the single familiar Gross-Pitaevskii equation. In general, due to the presence of the anomalous average, the unitary, nonlinear Schrödinger equation acquires a contribution proportional to the adjoint field α^*. Interestingly this leads to the breaking of time reversal symmetry.

To represent the equations compactly, it is useful to arrange them in a 2×2 matrix form. For convenience, we have transformed the field-equations to a frame co-rotating with a frequency μ defined by $\alpha(t) \rightarrow \exp(-i\mu t)\,\alpha(t)$. The generalized Gross-Pitaevskii equation is then given by

$$\frac{d}{dt}\begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix} = -i \begin{pmatrix} H^{(c)} - \mu & O^{(c)} \\ -O^{(c)*} & -(H^{(c)*} - \mu) \end{pmatrix} \begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix}. \tag{1}$$

The mean-field α evolves according to a non-hermitian Hamiltonian operator $H^{(c)}$ and interacts through the anomalous coupling strength $O^{(c)}$ with the adjoint field α^*

$$\begin{aligned} H^{(c)} &= H^{(0)} + 1\,U_{f^{(c)}} + 2\,U_{\tilde{f}} + i\,\Gamma^{(c)}_{\mathcal{N}}, \\ O^{(c)} &= V_{\tilde{m}} + i\,\Gamma^{(c)}_{\mathcal{A}}. \end{aligned} \tag{2}$$

While $H^{(0)}$ accounts for the free evolution, $U_{f^{(c)}}$, $U_{\tilde{f}}$ and $V_{\tilde{m}}$ arise from the self-interaction of the condensate and the mutual interaction with the normal and anomalous fluctuations, respectively. These operators, i.e.

$$\begin{aligned} U_f &= 2\,\phi^{1\,2'3'4'}\, f_{3'2'} \, |1\rangle \langle 4'|, \\ V_m &= 2\,\phi^{1\,2'3'4'}\, m_{3'4'} \, |1\rangle |2'\rangle, \end{aligned} \tag{3}$$

are defined explicitly in terms of the symmetrized ($\mathcal{S}$) two-body matrix elements that are derived from the binary interaction potential $V_{\rm bin}(\mathbf{x}_1 - \mathbf{x}_2)$

$$\begin{aligned} \phi^{1234} &= \frac{1}{2}(\mathcal{S})\, \langle 1| \otimes \langle 2|\, V_{\rm bin}(\mathbf{x}_1 - \mathbf{x}_2)\, |3\rangle \otimes |4\rangle, \\ \phi^{1234} &= \phi^{1243} = \phi^{2134} = \phi^{2143}. \end{aligned} \tag{4}$$

In addition to these first order contributions, the second order damping rates and

energy shifts are given by

$$\begin{aligned}\Gamma^{(c)}_{\mathcal{N}} &= \Gamma_{\tilde{f}\tilde{f}(1+\tilde{f})} + 2\Gamma_{\tilde{f}\tilde{m}\tilde{n}} - \Gamma_{(1+\tilde{f})(1+\tilde{f})\tilde{f}} - 2\Gamma_{(1+\tilde{f})\tilde{m}\tilde{n}},\\ \Gamma^{(c)}_{\mathcal{A}} &= 2\Gamma_{\tilde{f}\tilde{m}(1+\tilde{f})} - 2\Gamma_{(1+\tilde{f})\tilde{m}\tilde{f}} \quad .\end{aligned} \tag{5}$$

The individual collision processes that contribute to the total scattering rates into and out of the condensate are defined as

$$\begin{aligned}\Gamma_{fff} &= 8\,\phi^{1\,2'3'4'}\phi_\eta^{1''2''3''4''} f_{3'1''} f_{4'2''} f_{4''2'} \,|1\rangle\langle 3''|\,,\\ \Gamma_{fmf} &= 8\,\phi^{1\,2'3'4'}\phi_\eta^{1''2''3''4''} f_{3'1''} m_{4'3''} f_{4''2'} \,|1\rangle|2''\rangle\,,\\ \Gamma_{fmn} &= 8\,\phi^{1\,2'3'4'}\phi_\eta^{1''2''3''4''} f_{3'1''} m_{4'3''} n_{2''2'} \,|1\rangle\langle 4''|\,,\\ \Gamma_{mmn} &= 8\,\phi^{1\,2'3'4'}\phi_\eta^{1''2''3''4''} m_{3'4''} m_{4'3''} n_{2''2'} \,|1\rangle|1''\rangle\,.\end{aligned} \tag{6}$$

During a binary collision event, conservation of energy is not satisfied exactly in the Born-Markov approximation. Thus any second-order collision operator obtains a dispersive as well as a dissipative part from the complex matrix element

$$\phi_\eta^{1''2''3''4''} = \phi^{1''2''3''4''}\left(\pi\delta_\eta(\Delta_{1''2''3''4''}) + i\mathcal{P}_\eta\frac{1}{\Delta_{1''2''3''4''}}\right). \tag{7}$$

Here the matrix element is non-zero only if the energy difference $\Delta_{1''2''3''4''} = \varepsilon_{1''}(t)+\varepsilon_{2''}(t)-\varepsilon_{3''}(t)-\varepsilon_{4''}(t)$ between the initial and final single particle energies are within the energy shell of thickness η, as given by the limit

$$\lim_{\eta\to 0_+}\frac{1}{\eta - i\Delta} = \pi\,\delta_\eta(\Delta) + i\,\mathcal{P}_\eta\frac{1}{\Delta}. \tag{8}$$

where $\mathcal{P}$ defines the usual principal value contribution.

2.2 Normal and anomalous fluctuations

The normal and anomalous fluctuations of a quantum field are not independent quantities, but together they form a positive semi-definite co-variance matrix G

$$G = \begin{pmatrix}\tilde{f} & \tilde{m}\\ \tilde{n} & (1+\tilde{f})^{\top}\end{pmatrix} \geq 0. \tag{9}$$

Within the approximation of the kinetic theory, this co-variance matrix evolves as

$$\frac{d}{dt}G = -i\widetilde{\Sigma}\,G + i\,G\,\widetilde{\Sigma}^{\dagger} + I \tag{10}$$

with a non-hermitian second-order self-energy operator $\widetilde{\Sigma}$ and recycling terms I. In detail, this self-energy is

$$\widetilde{\Sigma} = \begin{pmatrix}\widetilde{H}-\mu & \widetilde{O}\\ -\widetilde{O}^* & -(\widetilde{H}^*-\mu)\end{pmatrix}, \tag{11}$$

where we have introduced non-hermitian Hamilton operators and anomalous coupling potentials;

$$\begin{aligned}\widetilde{H} &= H^{(0)} + 2\,U_{f^{(c)}} + 2\,U_{\tilde{f}} + i\,\widetilde{\Gamma}_{\mathcal{N}},\\ \widetilde{O} &= V_{(m^{(c)}+\tilde{m})} + i\,\widetilde{\Gamma}_{\mathcal{A}},\end{aligned} \tag{12}$$

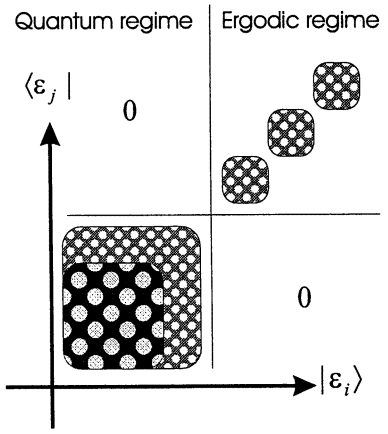

Figure 3. Schematic illustration of the quantum mechanical state space. In the lower energy region, the condensate (big circles), as well as the normal and anomalous fluctuations (small circles) overlap and interact coherently. Above this region in energy space ($\gg 2\mu$), there is the ergodic domain where energy levels are occupied incoherently.

collision rates;

$$\begin{aligned}
\widetilde{\Gamma}_{\mathcal{N}} &= \Gamma_{\tilde{f}\tilde{f}(1+\tilde{f})} + \Gamma_{\tilde{f}\tilde{f}f^{(c)}} + 2\Gamma_{f^{(c)}\tilde{f}(1+\tilde{f})} \\
&\quad - \Gamma_{(1+\tilde{f})(1+\tilde{f})\tilde{f}} - \Gamma_{(1+\tilde{f})(1+\tilde{f})f^{(c)}} - 2\Gamma_{f^{(c)}(1+\tilde{f})\tilde{f}} \\
&\quad + 2\Gamma_{\tilde{f}(m^{(c)}+\tilde{m})\tilde{n}} + 2\Gamma_{\tilde{f}\tilde{m}n^{(c)}} - 2\Gamma_{(1+\tilde{f})(m^{(c)}+\tilde{m})\tilde{n}} - 2\Gamma_{(1+\tilde{f})\tilde{m}n^{(c)}}, \\
\widetilde{\Gamma}_{\mathcal{A}} &= 2\Gamma_{\tilde{f}(m^{(c)}+\tilde{m})(1+\tilde{f})} + 2\Gamma_{f^{(c)}\tilde{m}(1+\tilde{f})} + 2\Gamma_{\tilde{f}\tilde{m}f^{(c)}} \\
&\quad - 2\Gamma_{(1+\tilde{f})(m^{(c)}+\tilde{m})\tilde{f}} - 2\Gamma_{f^{(c)}\tilde{m}\tilde{f}} - 2\Gamma_{(1+\tilde{f})\tilde{m}f^{(c)}}
\end{aligned} \tag{13}$$

and recycling terms;

$$I = \begin{pmatrix} I_{\tilde{f}} & -I_{\tilde{m}} \\ -I_{\tilde{m}}{}^{\dagger} & (I_{\tilde{f}} - \widetilde{\Gamma}_{\mathcal{N}} - \widetilde{\Gamma}_{\mathcal{N}}^{\dagger})^{\top} \end{pmatrix} \tag{14}$$

that correspond to feeding and loss;

$$\begin{aligned}
I_{\tilde{f}} &= \Gamma_{\tilde{f}\tilde{f}(1+\tilde{f})} + \Gamma_{\tilde{f}\tilde{f}f^{(c)}} + 2\Gamma_{f^{(c)}\tilde{f}(1+\tilde{f})} \\
&\quad + 2\Gamma_{\tilde{f}(m^{(c)}+\tilde{m})\tilde{n}} + 2\Gamma_{\tilde{f}\tilde{m}n^{(c)}} + 2\Gamma_{f^{(c)}\tilde{m}\tilde{n}} + \text{h.c.}, \\
I_{\tilde{m}} &= 2\Gamma_{\tilde{f}(m^{(c)}+\tilde{m})(1+\tilde{f})} + 2\Gamma_{\tilde{f}\tilde{m}f^{(c)}} + 2\Gamma_{f^{(c)}\tilde{m}(1+\tilde{f})} \\
&\quad + \left(2\Gamma_{(1+\tilde{f})(m^{(c)}+\tilde{m})\tilde{f}} + 2\Gamma_{(1+\tilde{f})\tilde{m}f^{(c)}} + 2\Gamma_{f^{(c)}\tilde{m}\tilde{f}}\right)^{\top} \\
&\quad + \Gamma_{\tilde{m}\tilde{m}(n^{(c)}+\tilde{n})} + 2\Gamma_{\tilde{m}m^{(c)}\tilde{n}} + \left(\Gamma_{\tilde{m}\tilde{m}(n^{(c)}+\tilde{n})} + 2\Gamma_{\tilde{m}m^{(c)}\tilde{n}}\right)^{\top}.
\end{aligned} \tag{15}$$

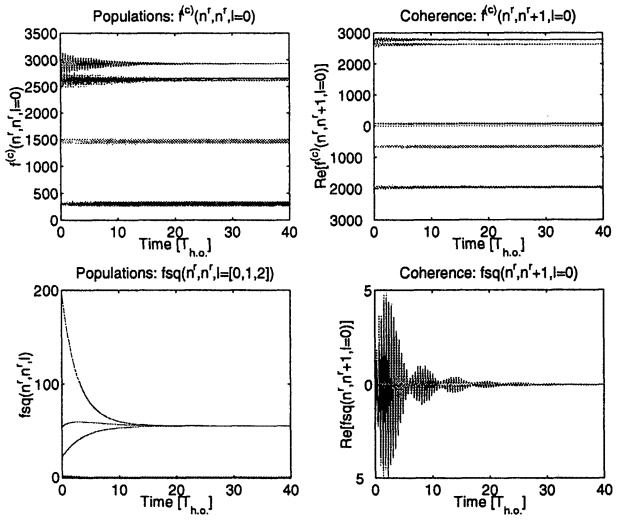

Figure 4. Real time evolution of the s-wave condensate interacting with the non-condensate. The upper two quadrants depict the populations $f^{(c)}_{n^r,n^r,l=0} = |\alpha_{n^r}|^2$ and the real part of the coherences $f^{(c)}_{n^r,n^r+1} = Re[\alpha_{n^r}\alpha^*_{n^r+1}]$ of the condensate as a function of time in units of the harmonic oscillator period $T_{\rm h.o} = 2\pi/\omega$. In the lower two segments, we show the corresponding populations $\tilde{f}_{n^r,n^r,l=0,2}$, and one set of off-diagonal elements $\tilde{f}_{n^r,n^r+1,l=0,2}$ of the normal fluctuations. The parameters used were the same as for Fig. 2.

3 Numerical solutions

To understand the implication of the quantum mechanical nature of the condensate interacting with the non-condensate fluctuations, it is necessary to solve these equations numerically. For simplicity, we assume a completely isotropic three-dimensional configuration, which makes it possible to decompose the equations in terms of angular momentum sub-manifolds. To study the low energy behavior, it is possible separate the state space into a quantum regime and an ergodic domain. We have illustrated this schematically in Fig. 3.

The first task in studying the dynamics of the system is to evolve the system in real time towards equilibrium. In Fig. 4, we show a characteristic trajectory that exemplifies the quantum mechanical nature of the solution. In particular, we have chosen a set of 3 interacting angular-momentum manifolds ($l = 0, 1, 2$) and used the lowest energy seven radial basis states ($n^r = 1 \ldots 7$ as illustrated in Fig. 2) to propagate the condensate and non-condensate.

As this simulation illustrates, while the populations relax towards their ergodic detailed balance solution, coherences persist for long times. The role of anomalous fluctuations and low energy coherences is determined from the form of the steady-state solution. Note that the theory here is a time-dependent one, and transient phenomena as well as the rate of phase diffusion of the broken symmetry can be investigated within our framework.

Acknowledgments

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