Reversible and irreversible evolution of a condensed bosonic gas

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We have formulated a kinetic theory for a condensed atomic gas in a trap, i.e., a generalized Gross-Pitaevskii equation, as well as a quantum-Boltzmann equation for the normal and anomalous fluctuations [R. Walser *et al.*, Phys. Rev. A **59**, 3878 (1999)]. In this paper, the theory is applied to the case of an isotropic configuration and we present numerical and analytical results for the reversible real-time propagation, as well as irreversible evolution towards equilibrium.

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I. INTRODUCTION

More than 70 years ago, Bose and Einstein proposed a provocative hypothesis—that at ultralow temperatures a novel state of matter should exist. They predicted this state could be attained by cooling an ordinary gas towards absolute zero. At a well-defined point in this process, a spontaneous transition should occur and change the state of matter from an unordered ensemble of individual particles into one collective entity. This single object, now devoid of its many-particle character, ought to evolve as a collective matter wave.

With the discovery of superfluidity in liquid helium in 1938 and its subsequent explanation in terms of Bose-Einstein condensation (BEC), the hypothesis had been firmly established. In turn, this phenomenon has had a major impact on the development of modern quantum physics. Today, BEC is fundamental to our understanding of many low-temperature phenomena and it is the cornerstone of many quantitative explanations. However, up to 1995, condensation of a weakly interacting, atomic Bose-Einstein gas had never been achieved, as such.

With the ground-breaking accomplishment of condensing atomic ^{87}Rb by Cornell and Wieman *et al.* [1], of sodium by Ketterle *et al.* [2], and lithium by Hulet *et al.* [3], a chapter of quantum statistical physics has been opened. It is now possible to study in a table-top experiment quantum statistical effects of material objects on a human scale (up to 5 mm—the very phenomena that govern the otherwise microscopic physics of nuclear matter, macroscopic quantum liquids, or astronomical objects, such as neutron stars.

Today, more bosonic alkali-metal elements have crossed the transition temperature, in particular atomic hydrogen [4] as well as ^{85}Rb [5], and many more vastly improved experiments have been carried out. For example, it is now possible to examine multicomponent condensates [6,7], to create vortices [8,9], and to prepare topological modes [10]. For a list of current experiments see Ref. [11], or the review article in Ref. [12]. However, the technological breakthrough of combining laser cooling with evaporative cooling is not limited to bosonic species only. Most recently, the fermionic isotope of potassium ^{40}K has also been cooled successfully below the Fermi temperature [13].

Instigated by these spectacular experiments, strongly renewed interest has developed in their quantitative description. While cold quantum gases had been studied extensively in the 1950–60's, they were mainly considered as precursor theories for strongly interacting systems, such as liquid helium. Thus, most of the available results were focused on spatially uniform systems in thermal equilibrium. Excellent accounts of these standard results can be found, for example, in the textbooks and monographs [14–19]. However, the spatial nonuniformity, the thermal isolation resulting from the confinement in a ultrahigh vacuum trap, as well as the large disparity of collision and relaxation time scales, are indispensable ingredients for a quantitative description of today's experiments.

To account for these differences that distinguish the present experimental situation from the homogeneous Bose-Einstein gas [20–23], a growing number of equilibrium and nonequilibrium kinetic theories have been recently presented [24–29]. However, the effort to go beyond the mean-field description of the Gross-Pitaevskii equation [30] is considerable. Thus, the research for a unified description of the equilibrium and nonequilibrium situation is still very active.

In this paper, we explore numerically and analytically some of the implications of the reversible and irreversible evolution of a condensed gas immersed in the noncondensate cloud. The points discussed are organized as follows. Section II revisits the main results of our kinetic theory [31], i.e., the two-particle Hamiltonian and the energy and number conserving collisional kinetic equations for the condensate, as well as the normal and anomalous fluctuations. In Sec. III, we specialize these kinetic equations for a completely isotropic situation. Based on these prerequisites, we discuss in Sec. IV the results of propagating the collisionless mean-field and the Hartree-Fock-Bogoliubov (HFB) equations in real time. Finally, in Sec. V, we study the evolution of an ergodic distribution towards equilibrium in the presence of collisions.

II. KINETIC MASTER EQUATIONS

A. Master variables

The kinetic master equation of the weakly interacting dilute atomic gas describes the coupled evolution of the condensed fraction immersed in the quantum fluctuations. In this context, we associate the condensate with a c number field $\alpha_{\mathbf{x}}(t)$ that represents the expectation value of the quantum

field $\langle \hat{a}_{\mathbf{x}}(t)\rangle$. The field operator $\hat{a}_{\mathbf{x}}$ removes a particle from point $\mathbf{x}$ and satisfies the scalar, equal-time commutation relation,

$$[\hat{a}_{\mathbf{x}},\hat{a}^{\dagger}_{\mathbf{y}}]=\delta(\mathbf{x}-\mathbf{y}), \tag{1}$$

of a boson. The position representation $\{|\mathbf{x}\rangle\}$ used above is not necessarily the most suitable basis to formulate a kinetic theory. It proves to be more useful to postpone the choice of a particular representation and to formulate the theory in terms of a general single-particle basis $\{|i_1\rangle\}$ that spans the same single-particle Hilbert space:

$$\hat{a}_{\mathbf{x}}=\sum_{i_1}\hat{a}_{i_1}\langle \mathbf{x}|i_1\rangle. \tag{2}$$

In the case of an unstructured (scalar) atomic condensate, three external quantum labels (i_1) are sufficient to describe its motional state in space, completely.[1] In this manner, we can expand any field as

$$\langle \hat{a}\rangle=\sum_{i_1}\alpha_{i_1}|i_1\rangle\equiv\alpha_1|1\rangle\equiv\alpha. \tag{3}$$

Here we have simplified the notation by dropping the name of the dummy variable, i.e., $i_1\equiv 1$, and by assuming implicit summation over repeated indices, as usual.

In an analogous fashion, we can describe the normal density of the atomic gas $f=\langle\hat{a}^{\dagger}\hat{a}\rangle=f^{(c)}+\tilde{f}$ by a Hermitian tensor operator of rank (1,1):

$$\tilde{f}=\tilde{f}_{12}|1\rangle\langle 2|,\quad f^{(c)}=\alpha_2^{*}\alpha_1|1\rangle\langle 2|. \tag{4}$$

Moreover, we will always decompose any quantum average into a mean-field contribution and the remaining fluctuations. Similarly, we define the anomalous averages $m=\langle\hat{a}\hat{a}\rangle=m^{(c)}+\tilde{m}$ as symmetric tensors of rank (2,0),

$$\tilde{m}=\tilde{m}_{12}|1\rangle|2\rangle,\quad m^{(c)}=\alpha_2\alpha_1|1\rangle|2\rangle, \tag{5}$$

and their symmetric conjugates as $n=m^{*}_{12}\langle 1|\langle 2|$.

B. Dynamical evolution

The kinetic evolution of a weakly interacting gas is primarily governed by the motion of the individual particles in the external trapping potential and by binary collisions. Simultaneous collisions of more than two particles are unlikely events in a dilute gas. Consequently, we will disregard such processes and use the following number-conserving Hamiltonian operator:

$$\hat{H}=\hat{H}^{(0)}+\hat{H}^{(1)}=H^{(0)^{12}}\hat{a}^{\dagger}_1\hat{a}_2+\phi^{1234}\hat{a}^{\dagger}_1\hat{a}^{\dagger}_2\hat{a}_3\hat{a}_4. \tag{6}$$

[1]This is readily generalized to accommodate multiple internal electronic configurations if i_1 encompasses more quantum labels accordingly, i.e., $|i_1\rangle=|n_1,l_1,m_1;F_1,M_1,\ldots\rangle$.

Here, $\hat{H}^{(0)}$ denotes a single-particle Hamiltonian operator with matrix elements $H^{(0)^{12}}=\langle 1|\mathbf{p}^2/(2m)+V_{\mathrm{ext}}(\mathbf{x})|2\rangle$. For the external trapping potential, we assume a three-dimensional isotropic harmonic oscillator, $V_{\mathrm{ext}}(\mathbf{x})=m\omega^2(x^2+y^2+z^2)/2$. In most of the present experiments with large, stable condensates, the two-body interaction potentials $V_{\mathrm{bin}}(\mathbf{x}_1-\mathbf{x}_2)$ are repulsive and of short range. From such potentials, we can obtain two-particle matrix elements as

$$\phi^{1234}=\frac{1}{2}(\mathcal{S})\langle 1|\otimes\langle 2|V_{\mathrm{bin}}(\mathbf{x}_1-\mathbf{x}_2)|3\rangle\otimes|4\rangle, \tag{7}$$

$$\phi^{1234}=\phi^{1243}=\phi^{2134}=\phi^{2143}. \tag{8}$$

Only the symmetric part of the two-particle matrix element ϕ^{1234} is physically relevant. Therefore, we have explicitly $(\mathcal{S})$ symmetrized it. In the low kinetic energy range that we are interested in, *s*-wave scattering is the dominant two-particle scattering event [32–34]. Thus, by discarding all details of the two-particle potential, we can describe the interaction strength with a single parameter V_0 related to the scattering length a_s by $V_0=4\pi\hbar^2 a_s/m$. This limit corresponds to a singular interaction potential, i.e., $V_{\mathrm{bin}}(\mathbf{x}_1,\mathbf{x}_2)=V_0\delta(\mathbf{x}_1-\mathbf{x}_2)$. In the case of this delta potential, one finds for the two-body matrix elements:

$$\phi^{1234}=\frac{V_0}{2}\int d^3\mathbf{x}\langle 1|\mathbf{x}\rangle\langle 2|\mathbf{x}\rangle\langle\mathbf{x}|3\rangle\langle\mathbf{x}|4\rangle, \tag{9}$$

which need not be symmetrized, as they are symmetric already. However, considering the caveats that are related to the singular functional form of the two-particle potential, [35], we will only rely on the existence and symmetry of the two-particle matrix elements as defined in Eq. (7).

C. Mean-field equations

Based on these assumptions, we have derived a set of kinetic equations that describe the dynamical evolution of the condensate fraction immersed in a cloud of noncondensate particles. By discarding all of the interactions except for the condensate's self-interaction, they reduce to the familiar Gross-Pitaevskii (GP) equation for the mean field α. However, due to the presence of anomalous fluctuations $\tilde{m}$, this nonlinear, but otherwise unitary GP equation acquires a contribution proportional to the time-reversed or complex conjugated field α^{*}.

To represent these equations compactly, it is useful to arrange them in a 2×2 matrix form. Moreover, we transform this field equation to a frame corotating with a positive frequency μ defined by $\alpha(t)=\exp(-i\mu t)\overline{\alpha}(t)$. However, in order not to overload the notation, we will suppress the overline in the following generalized GP equation:

$$\frac{d}{dt}\chi=(-i\Pi+\Upsilon^{<}-\Upsilon^{>})\chi. \tag{10}$$

The two-component state vector $\chi=(\alpha,\alpha^{*})^{\mathrm{T}}$, introduced above keeps track of the forward and time-reversed compo-

nents of the mean field. It is symmetric under time reversal, i.e., $\chi=\sigma_1\chi^*$. The Pauli matrix σ_1 achieves the exchange of upper and lower components and is defined in Appendix A.

Two distinct processes govern the real-time evolution of the mean field. First, there is the generalized GP propagator that is defined as

$$\Pi=\begin{pmatrix}\Pi_{\mathcal{N}} & \Pi_{\mathcal{A}}\\ -\Pi_{\mathcal{A}}^* & -\Pi_{\mathcal{N}}^*\end{pmatrix}. \tag{11}$$

The two contributions that define this symplectic propagator are a normal Hermitian Hamiltonian operator

$$\Pi_{\mathcal{N}}=H^{(0)}+1U_{f^{(c)}}+2U_{\tilde{f}}-\mu, \tag{12}$$

as well as a symmetric anomalous coupling strength

$$\Pi_{\mathcal{A}}=V_{\tilde{m}}. \tag{13}$$

It is easy to identify $\Pi_{\mathcal{N}}$ with the well-known unitary GP propagator that accounts for the free evolution of the mean-field $(H^{(0)}-\mu)$, its self-interaction $U_{f^{(c)}}$, as well as the energy shift $U_{\tilde{f}}$ caused by the presence of the noncondensate cloud. However, due to the existence of the anomalous fluctuations there is also a coupling through $\Pi_{\mathcal{A}}$ to the time-reversed field. For convenience, we have introduced two auxiliary operators U_f and V_m. Explicitly, they are defined in terms of the two-body matrix elements, such as

$$U_f=2\phi^{12'3'4'}f_{3'2'}|1\rangle\langle 4'|, \tag{14}$$

and a first-order anomalous coupling strength

$$V_m=2\phi^{12'3'4'}m_{3'4'}|1\rangle|2'\rangle. \tag{15}$$

Second, there are all of the collisional second-order damping rates and energy shifts [20–23] that are given by

$$\Upsilon^{<}=\begin{pmatrix}\Upsilon^{<}_{\mathcal{N}} & \Upsilon^{<}_{\mathcal{A}}\\ -\Upsilon^{>}_{\mathcal{A}}{}^* & -\Upsilon^{>}_{\mathcal{N}}{}^*\end{pmatrix}, \tag{16}$$

and the time-reversed contribution $\Upsilon^{>}=-\sigma_1\Upsilon^{<*}\sigma_1$. It can be shown that they are equivalent to the extended Beliaev rates [36].

The forward and backward transition rates $\Upsilon^{<}_{\mathcal{N}}$, $\Upsilon^{<}_{\mathcal{A}}$, $\Upsilon^{>}_{\mathcal{A}}$, and $\Upsilon^{>}_{\mathcal{N}}$, describe the bosonically enhanced scattering of noncondensate particles into and out of the condensate. In turn, these transition rates are formed from various binary scattering processes Γ, and are given by

$$\Upsilon^{<}_{\mathcal{N}}=\Gamma_{\tilde{f}\tilde{f}(1+\tilde{f})}+2\Gamma_{\tilde{f}\tilde{m}\tilde{n}}, \tag{17}$$

$$\Upsilon^{>}_{\mathcal{N}}=\Gamma_{(1+\tilde{f})(1+\tilde{f})\tilde{f}}+2\Gamma_{(1+\tilde{f})\tilde{m}\tilde{n}}, \tag{18}$$

and

$$\Upsilon^{<}_{\mathcal{A}}=\Gamma_{\tilde{m}\tilde{m}\tilde{n}}+2\Gamma_{\tilde{f}\tilde{m}(1+\tilde{f})}, \tag{19}$$

$$\Upsilon^{>}_{\mathcal{A}}=\Gamma_{\tilde{m}\tilde{m}\tilde{n}}+2\Gamma_{(1+\tilde{f})\tilde{m}\tilde{f}}. \tag{20}$$

Within the Born-Markov approximation of kinetic theory, we define these elemental collision processes as

$$\begin{aligned}
\Gamma_{fff}&=8\phi^{12'3'4'}\phi_\eta^{1''2''3''4''}f_{3'1''}f_{4'2''}f_{4''2'}|1\rangle\langle 3''|,\\
\Gamma_{fmf}&=8\phi^{12'3'4'}\phi_\eta^{1''2''3''4''}f_{3'1''}m_{4'3''}f_{4''2'}|1\rangle|2''\rangle,\\
\Gamma_{fmn}&=8\phi^{12'3'4'}\phi_\eta^{1''2''3''4''}f_{3'1''}m_{4'3''}n_{2''2'}|1\rangle\langle 4''|,\\
\Gamma_{mmn}&=8\phi^{12'3'4'}\phi_\eta^{1''2''3''4''}m_{3'4''}m_{4'3''}n_{2''2'}|1\rangle|1''\rangle.
\end{aligned} \tag{21}$$

During a binary collision event, two particles can conserve their energy only approximately. After all, the individual scattering event happens within a medium and the asymptotics cannot be reached within the finite duration of the collision. Thus, within the limits of the Born-Markov approximation, any second-order collision operator accrues a dispersive as well as a dissipative part from the complex valued matrix element:

$$\phi_\eta^{1''2''3''4''}=\phi^{1''2''3''4''}\frac{1}{\eta-i\Delta_{1''2''3''4''}}. \tag{22}$$

It is essentially nonzero only if the energy difference $\Delta_{1''2''3''4''}=\varepsilon_{1''}(t)+\varepsilon_{2''}(t)-\varepsilon_{3''}(t)-\varepsilon_{4''}(t)$ between the pre- and post-collision energies is smaller than an energy uncertainty η:

$$\lim_{\eta\to 0_+}\frac{1}{\eta-i\Delta}=\pi\delta_\eta(\Delta)+i\mathcal{P}_\eta\frac{1}{\Delta}. \tag{23}$$

On general physical grounds, it can be argued that this uncertainty η is bracketed by the binary collision rate, on one side, and the energy uncertainty arising from the finite duration of an individual collision event on the other side. As we have shown, one has also the liberty to choose a more accurate intermediate propagator such that the single-particle energies $\varepsilon(t)$ and the eigenstates incorporate mean-field shifts.

D. Normal and anomalous fluctuations

The normal and anomalous fluctuations $\tilde{f}(t)$ and $\tilde{m}(t)$ of a quantum field are not independent quantities, but actually they are the components a generalized single-time density operator $G^{>}(t)$:

$$G^{>}=\begin{pmatrix}\tilde{f} & \tilde{m}\\ \tilde{n} & (1+\tilde{f})^*\end{pmatrix}\geqslant 0. \tag{24}$$

The non-negativity of this covariance operator implies that the magnitude of the anomalous fluctuations is limited by the normal depletion through a Cauchy-Schwartz inequality (see Appendix B). In the general context of Green function's,[15,16] this single-time density operator $G^{>}(t)$ can also be viewed as a particular limit of a time-ordered $(\mathcal{T})$, two-time Green function $G(\tau,t)$, i.e., $G^{>}(t)=\lim_{\tau\to t_+}\mathcal{T}G(\tau,t)$. Consequently, it is also necessary to

consider the opposite limit and to define a time-reversed, single-time density operator through $G^{<}(t) = \lim_{\tau \to t_-} \mathcal{T}G(\tau,t)$. Explicitly, this operator is given by

$$G^{<} = \sigma_1 G^{>*} \sigma_1 = G^{>} + \sigma_3 = \begin{pmatrix} 1+\tilde{f} & \tilde{m} \\ \tilde{n} & \tilde{f}^* \end{pmatrix}. \tag{25}$$

With the help of these definitions, we can now present the results of the kinetic theory as a generalized Boltzmann equation for the single-time density operator $G^{>}(t)$ as

$$\frac{d}{dt} G^{>} = -i\Sigma G^{>} + \Gamma^{<} G^{<} - \Gamma^{>} G^{>} + \text{H.c.} \tag{26}$$

In analogy to the previous discussion of the mean-field dynamics, we again find that the evolution of the density operator is ruled by two types of propagators. First, there is the Hartree-Fock-Bogoliubov (HFB) self-energy operator Σ that can be obtained also by variational methods [16]. In detail, this symplectic self-energy is given by

$$\Sigma = \begin{pmatrix} \Sigma_{\mathcal{N}} & \Sigma_{\mathcal{A}} \\ -\Sigma_{\mathcal{A}}^* & -\Sigma_{\mathcal{N}}^* \end{pmatrix}, \tag{27}$$

where we have introduced Hermitian Hamiltonian operators and symmetric anomalous coupling potentials as

$$\Sigma_{\mathcal{N}} = H^{(0)} + 2U_{f^{(c)}} + 2U_{\tilde{f}} - \mu, \tag{28}$$

$$\Sigma_{\mathcal{A}} = V_{(m^{(c)}+\tilde{m})}. \tag{29}$$

It is important to note the different weighing factors of the mean-field potential in Eqs. (12) and (28), as well as the appearance of the anomalous condensate density $m^{(c)}$ in Eq. (29). This HFB operator is the usual starting point of any finite-temperature calculations. Depending on additional considerations, i.e., ''gapless vs conserving approximations'' (see Refs. [22] and [37–40]), the anomalous couplings $V_{\tilde{m}}$ are usually discarded from Eqs. (13) and (29). However, since we do go beyond a first-order calculation, we need to retain all contributions for consistency.

Second, the Boltzmann equation, Eq. (26), introduces forward and backward collision operators $\Gamma^{<}$ and $\Gamma^{>}$. They are responsible for particle transfer out of and into the condensate on one hand, and lead to thermal equilibration within the noncondensate cloud, on the other hand. These forward and backward collision operator are defined by

$$\Gamma^{<} = \begin{pmatrix} \Gamma_{\mathcal{N}}^{<} & \Gamma_{\mathcal{A}}^{<} \\ -\Gamma_{\mathcal{A}}^{>*} & -\Gamma_{\mathcal{N}}^{>*} \end{pmatrix}, \tag{30}$$

and $\Gamma^{>} = -\sigma_1 \Gamma^{<*} \sigma_1$, where

$$\Gamma_{\mathcal{N}}^{<} = \Gamma_{(\tilde{f}+f^{(c)})\tilde{f}(1+\tilde{f})} + \Gamma_{\tilde{f}f^{(c)}(1+\tilde{f})} + \Gamma_{\tilde{f}\tilde{f}f^{(c)}} + 2(\Gamma_{(\tilde{f}+f^{(c)})\tilde{m}\tilde{n}} + \Gamma_{\tilde{f}m^{(c)}\tilde{n}} + \Gamma_{\tilde{f}\tilde{m}n^{(c)}}), \tag{31}$$

$$\Gamma_{\mathcal{N}}^{>} = \Gamma_{(1+\tilde{f}+f^{(c)})(1+\tilde{f})\tilde{f}} + \Gamma_{(1+\tilde{f})f^{(c)}\tilde{f}} + \Gamma_{(1+\tilde{f})(1+\tilde{f})f^{(c)}} + 2(\Gamma_{(1+\tilde{f}+f^{(c)})\tilde{m}\tilde{n}} + \Gamma_{(1+\tilde{f})m^{(c)}\tilde{n}} + \Gamma_{(1+\tilde{f})\tilde{m}n^{(c)}}), \tag{32}$$

and

$$\Gamma_{\mathcal{A}}^{<} = \Gamma_{(\tilde{m}+m^{(c)})\tilde{m}\tilde{n}} + \Gamma_{\tilde{m}m^{(c)}\tilde{n}} + \Gamma_{\tilde{m}\tilde{m}n^{(c)}} + 2(\Gamma_{(\tilde{f}+f^{(c)})\tilde{m}(1+\tilde{f})} + \Gamma_{\tilde{f}m^{(c)}(1+\tilde{f})} + \Gamma_{\tilde{f}\tilde{m}f^{(c)}}), \tag{33}$$

$$\Gamma_{\mathcal{A}}^{>} = \Gamma_{(\tilde{m}+m^{(c)})\tilde{m}\tilde{n}} + \Gamma_{\tilde{m}m^{(c)}\tilde{n}} + \Gamma_{\tilde{m}\tilde{m}n^{(c)}} + 2(\Gamma_{(1+\tilde{f}+f^{(c)})\tilde{m}\tilde{f}} + \Gamma_{(1+\tilde{f})m^{(c)}\tilde{f}} + \Gamma_{(1+\tilde{f})\tilde{m}f^{(c)}}). \tag{34}$$

It is interesting to note that all of the collision processes that contribute to the Boltzmann equation, Eq. (26), are of the same basic structure as the collision operators in the GP equation, Eq. (10). In particular, one can generate all of the processes $\Gamma^{<}$ and $\Gamma^{>}$ by functional differentiation from $\Upsilon^{<}$ and $\Upsilon^{>}$. This very fact is actually the key principle to the functional-analytic Green functions method described in Ref. [15] and, for example, leads to the gapless Beliaev approximation [22,41].

E. Conservation laws

1. Number

The total particle number $\hat{N}$ is a conserved quantity if the atoms evolve under the generic two-particle Hamiltonian operator $\hat{H}$ given by Eq. (6), i.e., $[\hat{H},\hat{N}]=0$. This conservation law implies that the system is invariant under a global phase change $\hat{a} \to \hat{a}\exp(i\varphi)$. By using this continuous symmetry, i.e., $\alpha \to \alpha\exp(i\varphi)$, $\tilde{f} \to \tilde{f}$, and $\tilde{m} \to \tilde{m}\exp(2i\varphi)$, it is easy to see that kinetic Eqs. (10) and (26) are also explicitly number conserving at all times:

$$\langle \hat{N}(t) \rangle = \text{Tr}\{f^{(c)}(t)\} + \text{Tr}\{\tilde{f}(t)\} = \text{const.} \tag{35}$$

Nevertheless, it is important to note that there are always coherent and incoherent processes present that do transfer particles between the condensate and the noncondensate clouds, continuously.

2. Energy

In the absence of any time-dependent external driving fields, such as optical lasers or magnetic rf fields, the overall energy $\hat{H}$ must be conserved as well. To find the expectation value of the total system energy $E = \langle \hat{H} \rangle = \text{Tr}\{\hat{H}\sigma(t)\}$, one can use the same power-series expansion of the coarse-grained many-particle density matrix $\sigma(t)$ that leads to the kinetic equations. Thus, within the limits of the Born-Markov approximation and the systematic application of Wick's theorem, we have obtained first- and second-order contributions for the energy $E = \text{Tr}\{\hat{H}(\sigma^{(0)}_{\{\gamma(t)\}} + \sigma^{(1)}_{\{\gamma(t)\}})\} + O$ [3]. Explicitly, this energy functional $E = E^{(c)} + E[\tilde{f}] + E[\tilde{m}]$, is given as

$$E^{(c)}=\mathrm{Tr}\left\{\left[H^{(0)}+\frac{1}{2}[1U_{f^{(c)}}+2U_{\tilde{f}}+i(\Upsilon_{\mathcal{N}}^{<}-\Upsilon_{\mathcal{N}}^{>})]\right]f^{(c)}+\frac{1}{2}[V_{\tilde{m}}+i(\Upsilon_{\mathcal{A}}^{<}-\Upsilon_{\mathcal{A}}^{>})n^{(c)}\right\},\tag{36}$$

$$E[\tilde{f}]=\mathrm{Tr}\left\{\left[H^{(0)}+\frac{1}{2}[2U_{f^{(c)}}+2U_{\tilde{f}}+i(\Gamma_{\mathcal{N}}^{<}-\Gamma_{\mathcal{N}}^{>})]\right]\tilde{f}\right\},\tag{37}$$

$$E[\tilde{m}]=\mathrm{Tr}\left\{\frac{1}{2}[V_{m^{(c)}+\tilde{m}}+i(\Gamma_{\alpha}^{<}-\Gamma_{\mathcal{A}}^{>})]\tilde{n}\right\}.\tag{38}$$

For example, the same first-order results can be found in Ref. [16], derived by a variational procedure.

III. A COMPLETELY ISOTROPIC SYSTEM

In the previous section, we have reviewed the main results of the kinetic theory that describes the coupled evolution of the condensate immersed in the noncondensate. The formal derivation did not rely on a particular trapping geometry, nor a special form for the binary interaction potential. In order to gain deeper understanding of the intricate interactions, we will now specialize the theory to the most simple, though realistic, three-dimensional model: a completely isotropic configuration, a spherically symmetric harmonic trapping potential, and a binary short-range *s*-wave scattering potential.

A. Irreducible tensor fields

Complete isotropy is easily achieved for the mean field by decomposing it in terms of a few zero angular momentum partial waves. For this purpose, we will use a set of basis states $\{|1\rangle\}$ that can be characterized by radial and angular momentum quantum numbers (n,l,m), i.e., $\langle\mathbf{x}|1\rangle=R_{l_1}^{n_1}(r)Y_{m_1}^{l_1}(\theta,\varphi)$.

However, in order to isolate the isotropic components of the noncondensate fluctuations, $\tilde{f}$ and $\tilde{m}$, we need to generalize the concept of partial waves and introduce an irreducible set of tensor fields. Furthermore, by only selecting the scalar component $(l=0)$, we can enforce the desired radial symmetry. Thus, according to Refs. [42] and [43], we introduce irreducible representations of tensor fields of rank: (2,0), (1,1), (0,2) as

$$T_m^l(\overline{12})=\sum_{m_1,m_2}(-1)^{l_2-m_2}C_{m_1-m_2m}^{l_1l_2l}|n_1l_1m_1\rangle\langle n_2l_2m_2|,\tag{39}$$

$$S_m^l(\overline{12})=\sum_{m_1,m_2}(-1)^{l_2}C_{m_1m_2m}^{l_1l_2l}|n_1l_1m_1\rangle|n_2l_2m_2\rangle.$$

The quantum labels carry additional overlines or underlines to indicate whether a function depends only on two of the three quantum labels, for example, $\overline{1}\equiv(n_1,l_1)$ or $\underline{2}\equiv(l_2,m_2)$. With these definitions, it is easy to verify the following orthogonality relationships:

$$\mathrm{Tr}\{T_m^l(\overline{12})T_{m'}^{l'}(\overline{34})^{\dagger}\}=\delta_{\overline{13}}\delta_{\overline{24}}\delta_{ll'}\delta_{mm'},\tag{40}$$

$$\mathrm{Tr}\{S_m^l(\overline{12})S_{m'}^{l'}(\overline{34})^{\dagger}\}=\delta_{\overline{13}}\delta_{\overline{24}}\delta_{ll'}\delta_{mm'}.\tag{41}$$

In the case of a scalar field $(l=0)$, one can simplify Eq. (39) by the following relation for the Clebsch-Gordan coefficients $C_{m_1m_20}^{l_1l_20}=\delta_{l_1l_2}\delta_{m_1,-m_2}(-1)^{l_1-m_1}/\sqrt{2l_1+1}$. Provided the basis states transform under a coordinate rotation, here denoted by $\mathcal{R}$, according to the finite dimensional representation of the rotation group $\mathcal{D}^l(\mathcal{R})$ [43],

$$\mathcal{U}_{\mathcal{R}}|nlm\rangle=\sum_{m'}|nlm'\rangle\mathcal{D}_{m'm}^l(\mathcal{R});\tag{42}$$

it follows that the set of tensors $\{T_m^l\||m|\leqslant l\}$ and $\{S_m^l\||m|\leqslant l\}$ are irreducible as well:

$$\mathcal{U}_{\mathcal{R}}\otimes\mathcal{U}_{\mathcal{R}}{}^{-1}T_m^l(\overline{12})=\sum_{m'}T_{m'}^l(\overline{12})\mathcal{D}_{m'm}^l(\mathcal{R}),\tag{43}$$

$$\mathcal{U}_{\mathcal{R}}\otimes\mathcal{U}_{\mathcal{R}}S_m^l(\overline{12})=\sum_{m'}S_{m'}^l(\overline{12})\mathcal{D}_{m'm}^l(\mathcal{R}).\tag{44}$$

B. Isotropic two-particle matrix element

The most commonly used model for a short-range binary interaction potential is the *s*-wave hard-core delta potential $V_{\mathrm{bin}}(\mathbf{x}_1,\mathbf{x}_2)=V_0\delta(\mathbf{x}_1-\mathbf{x}_2)$. This model potential is most suited to describe the low energetic collision dynamics of two real particles. However, it has to be used with caution in connection with infinite summation over virtual, high-energy states. It is clear that the energy independent scattering approximation fails above a certain energy range when the spatial scale of variation of the high-energetic wave functions begin to sample the detailed form of the interaction potential. Thus, the true value of the interaction matrix element ought to decrease much faster with energy than the value obtained from the simple hard-core delta-potential approximation. It is well known that indiscriminate use of the energy independent approximation leads to a nonphysical ultraviolet divergence [28,35,44].

Considering these limitations, we will use the *s*-wave scattering matrix element that is obtained from the energy-independent approximation, i.e.,

$$\phi^{1234}=\frac{V_0}{2}\int_{-\infty}^{\infty}d^3\mathbf{x}\langle1|\mathbf{x}\rangle\langle2|\mathbf{x}\rangle\langle\mathbf{x}|3\rangle\langle\mathbf{x}|4\rangle,\tag{45}$$

only for energies below a certain level and truncate it appropriately otherwise.

By using the basis states $\langle\mathbf{x}|1\rangle=R_{l_1}^{n_1}(r)Y_{m_1}^{l_1}(\theta,\varphi)$, we can decompose the matrix element ϕ^{1234} into a reduced radial part $\phi^{\overline{1234}}$ and a purely geometric factor $Y^{\underline{1}\underline{2}\underline{3}\underline{4}}$,

$$\phi^{1234}=\phi^{\overline{1234}}Y^{\underline{1}\underline{2}\underline{3}\underline{4}},\tag{46}$$

where

$$\phi^{\overline{1234}}=\frac{V_0}{2}\int_0^\infty r^2 dr\, R_{l_1}^{n_1}(r)R_{l_2}^{n_2}(r)R_{l_3}^{n_3}(r)R_{l_4}^{n_4}(r) \quad (47)$$

and

$$Y^{\underline{1}\underline{2}\underline{3}\underline{4}}=\int d^2\Omega\, Y_{m_1}^{l_1^*}(\Omega)Y_{m_2}^{l_2^*}(\Omega)Y_{m_3}^{l_3}(\Omega)Y_{m_4}^{l_4}(\Omega)$$
$$=\sum_{l=0}^{\infty}\frac{C_{000}^{l_1l_2l}C_{000}^{l_3l_4l}C_{m_1m_2(m_1+m_2)}^{l_1l_2l}C_{m_3m_4(m_1+m_2)}^{l_3l_4l}}{4\pi(2l+1)\left(\prod_{i=1}^{4}(2l_i+1)\right)^{-1/2}}. \quad (48)$$

In the context of evaluating the collision integrals, it will be necessary to consider products of two matrix elements summed over all energetically accessible sublevels. Within the isotropic model, all magnetic sublevels are energetically degenerate. Moreover, spherical symmetry demands an equal population distribution and rules out the existence of coherences within magnetic submanifolds. Thus, it will be required to know the magnitude of $|Y^{\underline{1}\underline{2}\underline{3}\underline{4}}|^2$ averaged over all the magnetic quantum numbers. For later reference, we will now introduce such conveniently scaled factors as

$$g^{\overline{12}}=((2l_1+1)(2l_2+1))^{1/2}/2\pi, \quad (49)$$

$$g^{\overline{1234}}=2(\pi^2 g^{\overline{12}}g^{\overline{34}})^{-1}\sum_{m_1m_2m_3m_4}|Y^{\underline{1}\underline{2}\underline{3}\underline{4}}|^2$$
$$=2g^{\overline{12}}g^{\overline{34}}\sum_{l=0}^{\infty}\frac{(C_{000}^{l_1l_2l}C_{000}^{l_3l_4l})^2}{(2l+1)}. \quad (50)$$

These coupling strengths $g^{\overline{1234}}$ in Eq. (50) measure the amount and principle connectivity between precollision and post-collision angular momenta submanifolds $(l_3,l_4)\rightarrow(l_1,l_2)$. In particular, it establishes a parity selection rule such that the coefficients are nonvanishing only if the sum of the angular momenta is $l_1+l_2+l_3+l_4=$even. In addition, transitions are allowed only if the angular momentum l is within a range of $\max(|l_1-l_2|,|l_3-l_4|)\leqslant l\leqslant\min(l_1+l_2,l_3+l_4)$.

C. Scalar component of states and energies

With the help of the auxiliary results established in the previous section, we are now able perform the desired multipole decomposition of the kinetic equations. The postulate of complete isotropy then implies that we can focus on the scalar component of the field $(l=0)$ exclusively. This is

$$\alpha=\delta_{l,0}\delta_{m,0}\alpha_1|1\rangle, \quad \tilde{f}=\tilde{f}_{\overline{12}}T_0^0(\overline{12}),$$
$$\tilde{m}=\tilde{m}_{\overline{12}}S_0^0(\overline{12}), \quad \tilde{n}=\tilde{n}_{\overline{12}}S_0^{0\dagger}(\overline{12}). \quad (51)$$

Analogously, we can decompose all normal operators, such as the bare single-particle Hamiltonian operator, as

$$H^{(0)}=H_{\overline{14'}}^{(0)}T_0^0(\overline{14'}). \quad (52)$$

The first-order normal mean-field potential U_f and the anomalous coupling strength V_m are then

$$U_f=\phi^{\overline{12'}\,\overline{3'}\,\overline{4'}}g^{\overline{13'}}\delta_{l_2',l_3'}f_{\overline{3'2'}}T_0^0(\overline{14'}), \quad (53)$$

$$V_m=\phi^{\overline{12'}\,\overline{3'}\,\overline{4'}}g^{\overline{13'}}\delta_{l_3',l_4'}m_{\overline{3'4'}}S_0^0(\overline{12'}). \quad (54)$$

Finally, the normal and anomalous collisional contributions simplify to

$$\Gamma_{fff}=\phi^{\overline{12'}\,\overline{3'}\,\overline{4'}}\phi_\eta^{\overline{1''2''}\,\overline{3''4''}}g^{\overline{12'}\,\overline{3'}\,\overline{4'}}\delta_{l_3',l_1''}\delta_{l_4',l_2''}\delta_{l_4''l_2'}$$
$$\times f_{\overline{3'1''}}f_{\overline{4'2''}}f_{\overline{4''2'}}T_0^0(\overline{13''}), \quad (55)$$

$$\Gamma_{fmn}=\phi^{\overline{12'}\,\overline{3'}\,\overline{4'}}\phi_\eta^{\overline{1''2''}\,\overline{3''4''}}g^{\overline{12'}\,\overline{3'}\,\overline{4'}}\delta_{l_3',l_1''}\delta_{l_4',l_3''}\delta_{l_2''l_2'}$$
$$\times f_{\overline{3'1''}}m_{\overline{4'3''}}n_{\overline{2''2'}}T_0^0(\overline{14''}), \quad (56)$$

$$\Gamma_{fmf}=\phi^{\overline{12'}\,\overline{3'}\,\overline{4'}}\phi_\eta^{\overline{1''2''}\,\overline{3''4''}}g^{\overline{12'}\,\overline{3'}\,\overline{4'}}\delta_{l_3',l_1''}\delta_{l_4',l_3''}\delta_{l_4''l_2'}$$
$$\times f_{\overline{3'1''}}m_{\overline{4'3''}}f_{\overline{4''2'}}S_0^0(\overline{12''}), \quad (57)$$

$$\Gamma_{mmn}=\phi^{\overline{12'}\,\overline{3'}\,\overline{4'}}\phi_\eta^{\overline{1''2''}\,\overline{3''4''}}g^{\overline{12'}\,\overline{3'}\,\overline{4'}}\delta_{l_3',l_4''}\delta_{l_4',l_3''}\delta_{l_2''l_2'}$$
$$\times m_{\overline{3'4''}}m_{\overline{4'3''}}n_{\overline{2''2'}}S_0^0(\overline{11''}), \quad (58)$$

IV. REVERSIBLE EVOLUTION

In this section, we will examine several limiting situations of the reversible evolution in order to elucidate the complex behavior of the condensed gas. Since canonical transforms and Hartree-Fock-Bogoliubov (HFB) operators are crucial for an understanding of the reversible evolution, we will review the main results [16]. Subsequently, we are going to examine the stationary equilibrium, as well as the reversible real-time evolution of the condensed gas.

A. Structure of the generalized density matrix

The definition of a generalized density matrix G, i.e., either $G^>$ or $G^<$, was given in Eqs. (24) and (25). Its specific structure implies various important physical properties.

First of all, we have to assume that there is a basis that diagonalizes this $(2n\times 2n)$-dimensional fluctuation matrix. Exactly n of its $2n$ eigenvalues correspond to the positive occupation numbers of finding a particle or, more generally, a quasiparticle in a certain mode. For a given, but otherwise arbitrary, G matrix, one can construct this basis by studying the transformation law of the density matrix under a canonical transformation T (see Appendix A),

$$G'=TGT^\dagger. \quad (59)$$

It is important to note that this is not the transformation law of a general matrix under coordinate change. This would require that $T^\dagger=T^{-1}$. However, by only using the properties of the symplectic transformations, one can show that a canonical eigenvalue problem is defined by

$$(\sigma_3 G)T^\dagger = T^\dagger(\sigma_3 G'). \tag{60}$$

The solution of this eigenvalue problem yields the eigenvector matrix $T^\dagger$ and the corresponding diagonal eigenvalue matrix $\sigma_3 G'$. Here, we have introduced standard Pauli spin matrices σ_1 and σ_3, which exchange upper and lower component of a $2n$ dimensional vector, or flip the sign of the lower segment, respectively. All normalizable states can be rescaled such that $T\sigma_3 T^\dagger = \sigma_3$. Now, we are able to reconstruct the positive G matrix

$$G = VPV^\dagger, \tag{61}$$

from its eigenvectors $V = \sigma_3 T^\dagger$ and the diagonal, positive occupation number matrix $P = \sigma_3 G' \sigma_3$.

Second, an important feature of an admissible fluctuation matrix is its consistency with the commutation relation, i.e., $\langle \hat{a}_1 \hat{a}_2^\dagger \rangle = \langle \hat{a}_2^\dagger \hat{a}_1 \rangle + \delta_{12}$ and $\langle \hat{a}_1 \hat{a}_2 \rangle = \langle \hat{a}_2 \hat{a}_1 \rangle$. This can be expressed compactly as

$$\sigma_1 G^* \sigma_1 - G = \sigma_3. \tag{62}$$

By invoking the properties of a unitary symplectic transformation, one can show that the elements of the diagonal occupation number matrix P are not $2n$ independent variables. Actually half of them are determined by the other half, $P_{(n+1,\ldots,2n)} = 1 + P_{(1,\ldots,n)}$, or

$$\sigma_1 P \sigma_1 - P = \sigma_3. \tag{63}$$

In other words, by separating the occupation numbers P and the eigenvector matrix V into a first and second half, i.e., $(P_+, 1+P_+) = P$ and $(V_+, V_-) = V$, one can then decompose a general fluctuation matrix as

$$G = V_+ P_+ V_+^\dagger + V_-(1+P_+)V_-^\dagger. \tag{64}$$

B. Structure of the Hartree-Fock-Bogoliubov operator

The symplectic HFB operator arises not only naturally in kinetic theories or variational calculations, but in many other contexts involving stability analysis. In the case of bosonic fields, the self-energy operator is of the generic form:

$$\Sigma = \begin{pmatrix} \Sigma_{\mathcal{N}} & \Sigma_{\mathcal{A}} \\ -\Sigma_{\mathcal{A}}^* & -\Sigma_{\mathcal{N}}^* \end{pmatrix}. \tag{65}$$

In here, $\Sigma_{\mathcal{N}}$ stands for a Hermitian operator $\Sigma_{\mathcal{N}} = \Sigma_{\mathcal{N}}^\dagger$ and $\Sigma_{\mathcal{A}}$ denotes an anomalous coupling term that has to be symmetric $\Sigma_{\mathcal{A}} = \Sigma_{\mathcal{A}}^{\mathsf{T}}$. The relative size of the operators $\Sigma_{\mathcal{N}}$ and $\Sigma_{\mathcal{A}}$ determines the character of the energy spectrum. It can either be real valued with pairs of positive and negative eigenenergies, or one finds a doubly degenerate zero eigenvalue, if the energy difference between the smallest positive and highest negative vanishes (gapless spectrum). In the general case, there is a mixed spectrum consisting of pairs of real sign reversed as well as pairs of complex conjugated eigenvalues. The eigenvectors W are normalizable with respect to the indefinite norm $\|W\|^2 = W^\dagger \sigma_3 W$, except for those that belong to zero or complex eigenvalues. It is important to note that this energy basis W is in general distinct from the instantaneous basis V that diagonalizes the fluctuation matrix G in Eq. (61). They do coincide only in equilibrium. The mathematical properties of the eigenstates W can be derived easily from the intrinsic symmetries of the HFB operator:

$$\Sigma = -\sigma_1 \Sigma^* \sigma_1, \tag{66}$$

$$\Sigma^\dagger = \sigma_3 \Sigma \sigma_3. \tag{67}$$

Thus, if W and E are the solutions of the right eigenvalue problem,

$$\Sigma W = WE, \tag{68}$$

it follows directly from Eq. (66) that $\overline{W} = \sigma_1 W^*$, is also a right eigenvector but corresponds to the eigenvalue $\overline{E} = -E^*$. Starting from the second symmetry in Eq. (67) and the right eigenvalue problem of Eq. (68), it is easy to construct the left eigenvectors $\widetilde{W} = W^\dagger \sigma_3$ that correspond to the eigenvalues $\widetilde{E} = E^*$:

$$\widetilde{W}\Sigma = E^* \widetilde{W}. \tag{69}$$

Finally, from a combination of the results for the right and left eigenvectors, it follows that the eigenvectors are orthogonal with respect to the metric σ_3:

$$0 = (E^* - E')W_E^\dagger \sigma_3 W_{E'}, \tag{70}$$

if $E^* \neq E'$. On the other hand, this relation implies also that eigenvectors that belong to complex eigenvalues must have zero norm.

The situation of a doubly degenerate zero-energy eigenvalue $E = 0$ needs special attention. One can view this case as a limit when two nondegenerate states approach each other. However, as the energy gap decreases, the two eigenstates become more and more collinear. Thus, in the limit of a vanishing energy separation, the dimension of the spanned vector space collapses from 2 to 1 and Σ becomes defective. In the present context however, we did not encounter this situation (see Ref. [16] for details).

C. Stationary solution of the Hartree-Fock-Bogoliubov equations

In spite of the complex nonlinear interactions taking place within the atomic gas, the kinetic evolution is completely reversible if we disregard all collisionally induced redistributions of quasiparticles. Thus, for the moment, we will eliminate the collision operators Υ and Γ from the kinetic Eqs. (10) and (26) and we will study the collisionless stationary equilibrium, as well as the real-time evolution in this section.

With these assumptions, we are left with the following set of stationary equations for the mean field χ and the fluctuations $G^>$:

$$0 = \Pi \chi, \tag{71}$$

$$0 = \Sigma G^> - G^> \Sigma^\dagger. \tag{72}$$

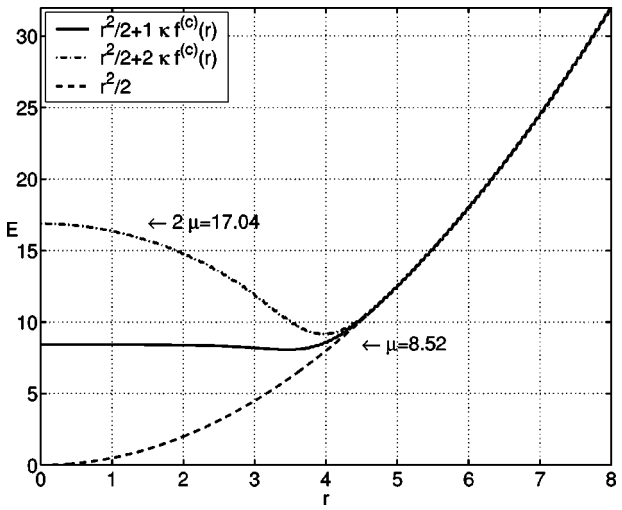

FIG. 1. Self-consistent potential energy densities of the condensate Hamilton operator $\Pi_{\mathcal{N}}$ (solid), the noncondensate Hamilton operator $\Sigma_{\mathcal{N}}$ (dashed dot), and the bare harmonic-oscillator potential (dashes) versus radius. Energy and length are scaled in the natural units for a harmonic oscillator.

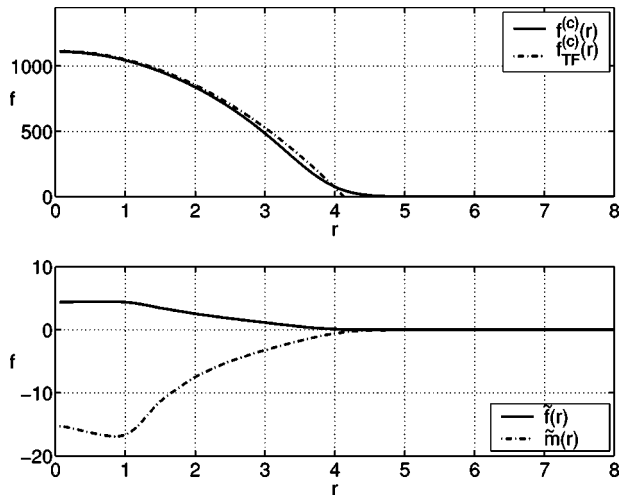

FIG. 2. Position density of the mean-field $f^{(c)}(r)$ (solid), the Thomas-Fermi approximation $f^{(c)}_{\mathrm{TF}}(r)$ (dashed-dot), as well as the normal fluctuations $\tilde{f}(r)$ (solid) and the anomalous fluctuations $\tilde{m}(r)$ (dashed-dot). Density and length are scaled in the natural units for a harmonic oscillator.

The self-energies of the condensate Π and the noncondensate Σ are nonlinearly coupled and implicitly include the rotation frequency of the mean-field μ.

However, the equilibrium solution to Eqs. (71) and (72) is not fully determined as it stands. From the results of the previous section, we know that any fluctuation matrix $G^{>}$ that is diagonal with respect to the positive and negative energy eigenvectors $W=(W_+,W_-)$ of Σ, will be a stationary and complete solution of Eq. (72)

$$G^{>}=W_+P_+W_+^{\dagger}+W_-(1+P_+)W_-^{\dagger}. \tag{73}$$

By choosing a canonical Bose-Einstein distribution $P(E>E_0)=1/[\exp(\beta E)-1]$ for the quasiparticles above the nondegenerate ground state $E_0>0$ and a vanishing ground-state occupation number $P(E_0)=0$, we obtain a variationally minimal energy solution for the total system at some inverse temperature β [16].

$$G^{>}=\sum_{E\geq E_0} P(E)W_EW_E^{\dagger}+[1+P(E)]W_{-E}W_{-E}^{\dagger}. \tag{74}$$

In order to understand the self-consistent equilibrium solution of Eqs. (71) and (72), it is useful to examine first the potentials that govern the evolution of the condensate, as well as the noncondensate. In Fig. 1, we depict the potential energy densities of the normal Hamiltonian operators $\Pi_{\mathcal{N}}$ and $\Sigma_{\mathcal{N}}$ versus radius that arise for the zero angular momentum manifold $l=0$, i.e., $V_{\mathrm{ext}}+1U_{f^{(c)}}$ and $V_{\mathrm{ext}}+2U_{f^{(c)}}$, respectively. They are compared to the bare isotropic harmonic-oscillator potential $V_{\mathrm{ext}}=r^2/2$, for reference. Here and in all of the subsequent results, we will use the experimental data of a typical ^{87}Rb condensate [45]. All physical parameters are scaled in the natural units for a harmonic oscillator, i.e., the angular frequency $\omega=2\pi 200\,\mathrm{Hz}$, the atomic mass $m_{87}=86.9092\,\mathrm{amu}$, the ground-state size $a_H=[\hbar/(\omega m_{87})]^{1/2}=763\,\mathrm{nm}$, the s-wave scattering length $a_S=5.82\,\mathrm{nm}=7.63\times10^{-3}a_H$, a very low temperature of $k_BT=0.2\hbar\omega$, and a condensate number chosen as $N^{(c)}=10^4$. The isotropic particle densities are normalized to $N=\int_0^{\infty}dr\,r^2\,f(r)$. From the effective coupling parameter $\kappa=a_S/a_H$, one obtains an estimate of the mean-field energy shift as $\mu_{\mathrm{TF}}=(15N^{(c)}\kappa)^{2/5}/2=8.36$. This gives an excellent approximation of the self-consistent chemical potential of $\mu=8.52$, as can be seen in Fig. 1.

The position densities of the condensate $f^{(c)}(r)$, as well as the local densities of the normal and anomalous fluctuations, i.e., $\tilde{f}(r)$ and $\tilde{m}(r)$, are represented in Fig. 2. First of all, it has to be noted that the solutions are real valued. This important fact follows from the detailed structure of the stationary Eqs. (71) and (72), which are invariant under a global phase change. Second, if we focus on the condensate density, one can see that it closely follows the Thomas-Fermi approximation $f^{(c)}_{\mathrm{TF}}(r)=(r^2_{\mathrm{TF}}-r^2)/(2\kappa)$, for radii less than $r_{\mathrm{TF}}=\sqrt{2\mu}\approx4.12$. This limit is valid in the strong-coupling regime $N^{(c)}\kappa>1$, where the kinetic energy is a negligible contribution compared to the external trapping potential and the self-energies. The self-consistent solutions for the normal and anomalous densities are depicted in the lower half of Fig. 2. While all normal densities are necessarily positive, the anomalous fluctuations carry a negative sign. The anomalous fluctuations are the response of the noncondensate medium to a phase-coherent mean field. In analogy to the polarization of an atom that is subjected to an electric field, it tries to compensate for the external perturbation. In the evaluation of the normal and anomalous fluctuations, we have truncated the finite-temperature sums beyond the radial and angular momentum quantum numbers $n^r=14$ and $l=6$. This leads to fully converged values of the normal fluctuations. However, it has to be noted that the values of the anomalous fluctuations are still subject to change (further decrease). As long as one keeps adding vacuum contribu-

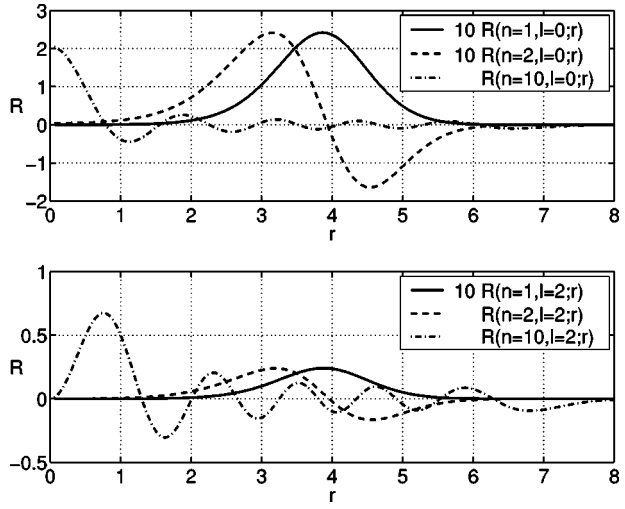

FIG. 3. Radial eigenfunctions $R_l^{n^r}(r)$ of the particlelike basis states $|\tilde{1}\rangle$ associated with the noncondensate Hamiltonian operator $H^{(0)}+2U_{f^{(c)}}$ versus radius. Depicted are a few representative states for the radial and angular quantum numbers $n^r=1, 2, 10$ and $l=0,2$.

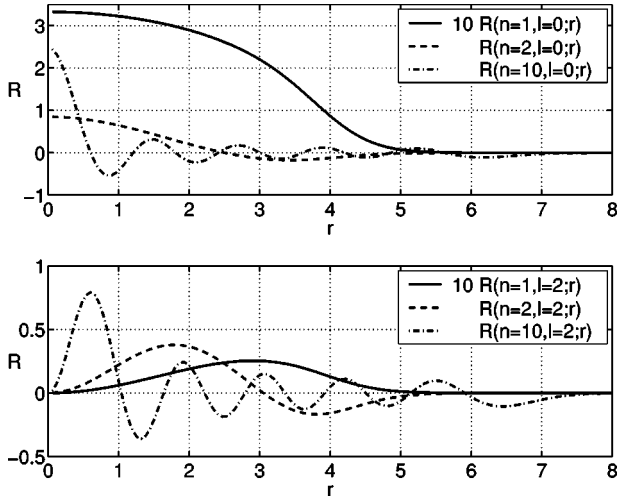

FIG. 4. Radial eigenfunctions $R_l^{n^r}(r)$ of the phononlike basis states $|1^{(c)}\rangle$ of the mean-field Hamiltonian operator $H^{(0)}+1U_{f^{(c)}}$ versus radius. Depicted are a few representative states for the radial and angular quantum numbers $n^r=1$, 2, 10, and $l=0,2$.

tions at an unaltered strength of the *s*-wave matrix-element $\phi^{n_1^r l_1 n_2^r l_2 n_3^r l_3 n_4^r l_4}$ [see Eq. (46)], this would lead to the well known ultraviolet divergence [28,35,44]. Thus, a judicious truncation, or alternatively an energy renormalization is needed to remove the nonphysical divergence that arises solely from the energy-independent approximation of the scattering amplitudes.

In Fig. 3, we show a few selected radial eigenfunctions $\langle \mathbf{x}|\tilde{1}\rangle = R_l^{n^r}(r)Y_m^l(\theta,\varphi)$ of the noncondensate Hamiltonian operator $(H^{(0)}+2U_{f^{(c)}})|\tilde{1}\rangle=\varepsilon_1|\tilde{1}\rangle$. The lowest energy state $R_{l=0}^{n^r=1}(r)$ is localized at the rim of the condensate $r_{\mathrm{TF}}=\sqrt{2\mu}\approx 4.12$. It has a smaller spatial extent than the condensate and consequently a higher energy. All *s*-wave functions ($l=0$) have a finite value at the origin in contrast to the $l>0$ states that must be vanishing at $r=0$. An eigenfunction that is characterized by quantum numbers (n^r,l) has n^r-1 nodes. Eigenfunctions corresponding to higher angular momenta l are shifted outwards due to the increased angular momentum barrier $l(l+1)/r^2$. The corresponding eigenenergies are depicted in Fig. 5. In the context of spatially homogeneous condensed matter systems, these eigenfunctions are associated with particlelike excitations.

The other relevant set of eigenstates arises from the condensate Hamiltonian operator, i.e., the stationary GP equation $(H^{(0)}+1U_{f^{(c)}})|1^{(c)}\rangle=\varepsilon_1|1^{(c)}\rangle$. The lowest self-consistent energy eigenstate defines the condensate wave function. A selection of these eigenstates are shown in Fig. 4. As these states correspond to the low energetic excitation modes of the condensate they are referred to as phononlike. The eigenenergies of the isotropic ($l=0$) modes are shown in Fig. 5.

We have compiled the four important positive energy spectra that arise in the problem in Fig. 5. In essence, these are the spectra of the condensate and the noncondensate Hamiltonians, $\Pi_{\mathcal{N}}$ and $\Sigma_{\mathcal{N}}$, as well as their generalization in terms of the HFB self-energy operators Π and Σ. It can be seen that the *s*-wave energies of $\Pi_{\mathcal{N}}$ and Π are virtually identical. In contrast to this, one finds that the excitation frequencies of the fluctuations Σ are characteristically shifted downwards from the energies of the noncondensate $\Sigma_{\mathcal{N}}$. It is also important to note that the self-energy of the fluctuations $\Sigma_{\mathcal{N}}$ includes the energy shifts of the noncondensate itself. These numerical results compare well within the limits of validity with the perturbative and semiclassical approximations of Refs. [46–48].

The spectrum of eigenvalues of Σ exhibits a characteristic energy gap above the condensate energy level μ. It is well known that this gap energy vanishes asymptotically for a

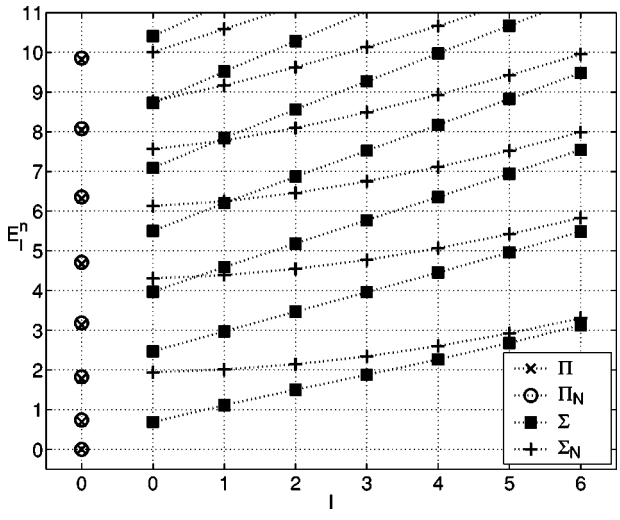

FIG. 5. Energy spectra $E_l^{n^r}$ versus radial and angular quantum numbers $1\leqslant n^r\leqslant 8$ and $0\leqslant l\leqslant 6$ for the phononlike states of $\Pi_{\mathcal{N}}$ ($l=0$, only), the particlelike states of $\Sigma_{\mathcal{N}}$, as well as the positive part of the energy spectrum of Π ($l=0$, only) and HFB self- energy Σ. Dimensionless energies are measured in natural harmonic-oscillator units.

homogeneous system in the thermodynamic limit. By deliberately excluding the anomalous coupling $V_{\tilde{m}}$ strength from a first-order theory (Popov approximation) or by including the second-order Beliaev correction of Eq. (26) in the self-energies, one can obtain a gapless approximation [22].

D. Time-dependent solution of the Hartree-Fock-Bogoliubov equations

After studying some aspects of the stationary solutions of the generalized HFB equations Eqs. (71) and (72), such as the local densities, the eigenstates, or the energy spectra, we will now investigate the reversible real time evolution of the coupled condensate and noncondensate system, i.e.,

$$\frac{d}{dt}\chi = -i\Pi\chi, \tag{75}$$

$$\frac{d}{dt}G^{>} = -i\Sigma G^{>} + iG^{>}\Sigma^{\dagger}. \tag{76}$$

In contrast to the complete kinetic Eqs. (10) and (26), which account for collisionally induced energy shifts and irreversible population transfer, Eqs. (75) and (76) contain only the first-order reversible processes. As we will show in the following, this restriction implies constant occupation numbers P.

In Sec. IV A, we have shown that any admissible fluctuation matrix $G^{>}$ has to be of the form

$$G^{>} = V_{+}PV_{+}^{\dagger} + V_{-}(1+P)V_{-}^{\dagger}, \tag{77}$$

where P represents the positive occupation numbers of the eigenstates V_{+}. This property is not only to be satisfied in equilibrium where the eigenstates coincide with the HFB states [see Eq. (74)], but in all instances.

By formally integrating the reversible kinetic equations, we can show that this structure of the fluctuation matrix is preserved at all times. Thus, Eqs. (75) and (76) define a consistent initial value problem. This simple but important fact can be demonstrated easily by defining the formal solution in terms of a time-ordered exponential:

$$T(t,t_0) = \mathcal{T}\exp\left[-i\int_{t_0}^{t} dt'\Sigma(t')\right]. \tag{78}$$

It is obvious that the propagator matrix $T(t,t_0)$ can be constructed in two steps by $T(t,t_0)=T(t,t_1)T(t_1,t_0)$ since the self-energy is local in time (semigroup property). Moreover, it follows from the structure of the generator that $T(t,t_0)$ is a proper symplectic transformation $\sigma_3 = T(t,t_0)\sigma_3 T(t,t_0)^{\dagger}$ at all times. Consequently, all occupation numbers of the general solution to the nonlinear, initial value problem are constants of motion

$$\begin{aligned} G^{>}(t) &= T(t,t_0)G^{>}(t_0)T(t,t_0)^{\dagger} \\ &= V_{+}(t)P(t_0)V_{+}^{\dagger}(t) + V_{-}(t)(1+P(t_0))V_{-}^{\dagger}(t), \end{aligned} \tag{79}$$

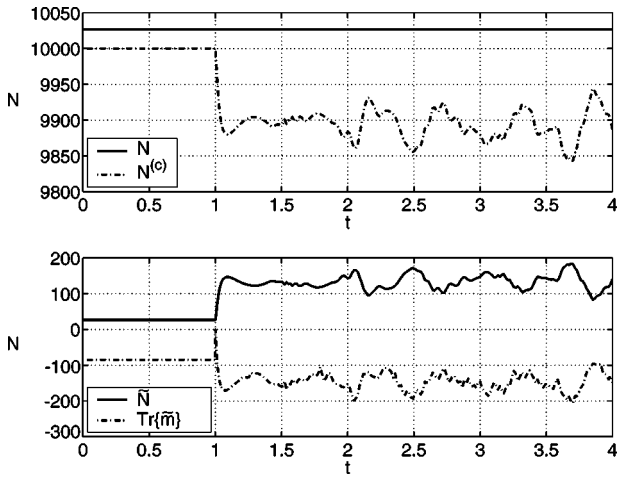

FIG. 6. Real-time evolution of the total particle number $N = N^c + \tilde{N}$ (solid), the number of particles in the condensate N^c (dash-dot), the noncondensate particles number $\tilde{N}$ (solid) and the trace over the anomalous fluctuations $\mathrm{Tr}\{\tilde{m}\}$ (dashed-dot). At $t=1$, the equilibrium solution is suddenly distorted by setting $\tilde{m}(t=1)=0$. Dimensionless time is measured in natural harmonic-oscillator periods.

with time-evolved basis states $V(t)=T(t,t_0)V$. Since $T(t,t_0)$ represents a genuine symplectic transform, the eigenstates $V^{\dagger}(t)\sigma_3 V(t) = V^{\dagger}\sigma_3 V = \sigma_3$ remain orthogonal.

In the following figures, we illustrate these fundamental facts that effectively define reversibility for any nonlinear system in the generic form of Eqs. (75) and (76). In particular, we will use the self-consistent, finite-temperature solution for $\chi(t=0)=\chi(\beta)$ and $G^{>}(t=0)=G^{>}(\beta)$ as an initial value for the time propagation at $t=0$. It is obvious that this choice does not induce any change during the subsequent real-time evolution. However, at $t=1$, we suddenly distort this equilibrium solution by setting the anomalous component of $G^{>}(t=1_{-})$ to zero, i.e., $\tilde{m}(t=1_{+})=0$ and then propagate forward up to $t=4$. It is important to note that the new $G^{>}(t=1_{+})$ is still a valid fluctuation matrix.

In Fig. 6, we have depicted the number of particles that occupy the condensate $N^{(c)}=\mathrm{Tr}\{f^{(c)}(t)\}$, the noncondensate $\tilde{N}=\mathrm{Tr}\{\tilde{f}(t)\}$, and the total particle number $N=N^{(c)}+\tilde{N}$ versus time. Time is measured in units of the harmonic-oscillator period $T=2\pi/\omega$. In contrast to these numbers that are genuine single-particle properties, the anomalous fluctuations are a physical measure of the degree of two-particle correlations or squeezing.[49] For example, the total particle number fluctuations $\langle(\hat{N}-\langle\hat{N}\rangle)^2\rangle$ or, more specifically, the normally ordered density fluctuations $\langle{:}\hat{f}(\mathbf{x},\mathbf{x}),\hat{f}(\mathbf{y},\mathbf{y}){:}\rangle$ would reflect the degree of squeezing of the quadrature components along certain directions $\mathbf{x},\mathbf{y}$. While we have not evaluated such observables here, we have included the averaged strength of the anomalous fluctuations $\mathrm{Tr}\{\tilde{m}\}$ to represent their size.

The most important feature in Fig. 6 is the exact conservation of the total particle number during all phases of the evolution. The instantaneous change in $\tilde{m}(t=1)$ does not affect it directly. But it can be seen that the relative partition-

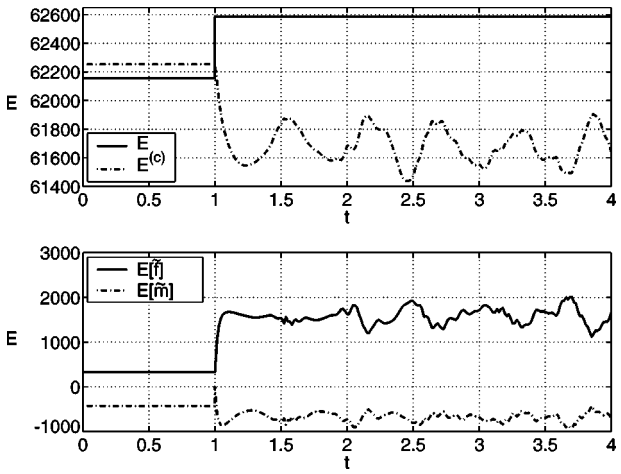

FIG. 7. Real-time evolution of the total system energy $E=E^{(c)}+E[\tilde{f}]+E[\tilde{m}]$ (solid), the energy of the particles in the condensate $E^{(c)}$ (dashed-dot), the normal noncondensate energy $E[\tilde{f}]$ and the anomalous energy $E[\tilde{m}]$. At $t=1$, the equilibrium solution is suddenly distorted by setting $\tilde{m}(t=1)=0$. Dimensionless energy is measured in natural harmonic oscillator units.

ing of the particles between condensate and normal noncondensate is massively distorted by this sudden influx of energy and particles start to oscillate coherently between the coupled subsystems.

In Fig. 7, we show the individual first-order contributions to the total system energy $E=E^{(c)}+E[\tilde{f}]+E[\tilde{m}]$ as described in Eqs. (36)–(38). Again the most notable feature is the exact conservation of total energy during the time evolution. Due to the sudden change in the anomalous fluctuations at $t=1$, the overall energy increases instantaneously by more than 400 $\hbar\omega$.

In Fig. 8, we show the complete spectrum of occupation numbers $P(1\leqslant n^r\leqslant 14,0\leqslant l\leqslant 6;t)$ that occur in the instantaneous fluctuation matrix $G^{>}(t)$, as defined by Eq. (79).

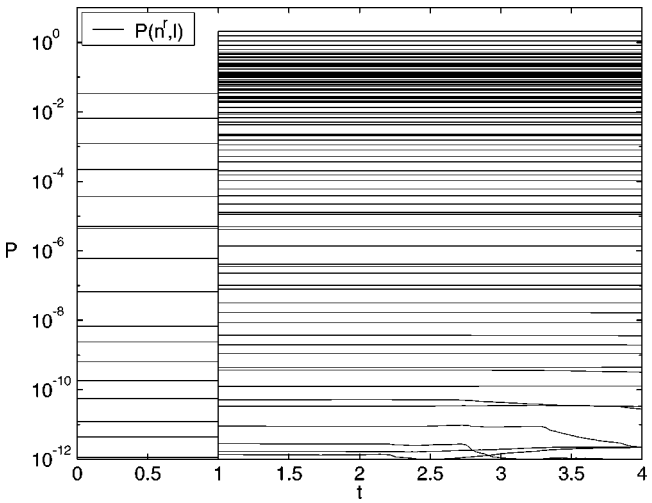

FIG. 8. Real-time evolution of the instantaneous occupation numbers $P(1\leqslant n^r\leqslant 14,0\leqslant l\leqslant 6)$ that characterize the fluctuation matrix $G^{>}(t)$. At $t=1$, $G^{>}(t)$ is suddenly distorted by setting $\tilde{m}(t=1)=0$.

From the logarithmic plot that covers 13 decades, it can be seen that the occupation numbers are indeed numerically exact constants of motion. Due to the instantaneous change at $t=1$, many of the high-energy occupation numbers that are quasidegenerate before the change, split up into a multitude of nondegenerate levels afterwards. Minute changes in the occupation numbers $|\delta P|<10^{-10}$ at the end of the integration period identify the precision loss of the numerical calculation.

The numerical results discussed in this section were obtained by discretizing the generalized GP Eq. (75) and the reversible part of the Boltzmann Eq. (76) with a standard finite element method [50] based on *b*-splines [51,52]. The use of these finite-support, piecewise polynomial basis functions results in matrix representations of the kinetic and potential energy operators that are banded. Very efficient linear algebra algorithms can be employed in this case [LAPACK (Ref. [53])]. In particular, we used a set of 400 *b*-splines on an equidistant radial grid from $0\leqslant r\leqslant 25\approx 6r_{\mathrm{TF}}$. Eventually, we represented the condensate wave function α (Fig. 2), the particlelike basis states $|\tilde{1}\rangle$ (Fig. 3), as well as the phononlike basis states $|1^{(c)}\rangle$ (Fig. 4) in this *b*-spline basis. Finally, a subset of quantum states was chosen (either $|\tilde{1}\rangle$ or $|1^{(c)}\rangle$) with $\{(n^r\geqslant 1,l\geqslant 0):2(n^r-1)+l<=18\approx 2\mu\}$ to evaluate the finite-temperature sums or to propagate in real time. We have verified numerically that no particular advantage can be obtained from either choice, as long as all of the relevant energies scales are resolved. The conservation of the total particle number $\langle N\rangle$ (Fig. 6), the total energy E (Fig. 7) as well as the instantaneous occupation numbers P (Fig. 8) support this argument.

V. THE IRREVERSIBLE EVOLUTION

A. An ergodic equilibrium solution of the master equation

In the following discussion of the irreversible evolution of the kinetic equations, we will again try to elucidate the main physics by additional simplifications. In particular, we will assume ergodicity for the normal fluctuations $\tilde{f}_{12}=\delta_{12}\tilde{f}_{\varepsilon_1}$, and the anomalous fluctuations $\tilde{m}=0$. This physical approximation is appropriate for most kinetic temperatures, except for a region close to $T=0$. Within this limit, we are able to establish an important result for the stationary behavior of the condensed atomic gas, i.e., a canonical Bose-Einstein distribution for the noncondensate particles coexisting with an energetically lower-lying, coherent condensate mode. By imposing the restriction of vanishing anomalous fluctuations upon the kinetic equations, [Eqs. (10) and (26)], we are left with the following equations of motion:

$$\frac{d}{dt}\alpha=(-i\Pi_{\mathcal{N}}+\Upsilon^{<}_{\mathcal{N}}-\Upsilon^{>}_{\mathcal{N}})\alpha, \tag{80}$$

$$\frac{d}{dt}\tilde{f}=\Gamma^{<}_{\mathcal{N}}(1+\tilde{f})-\Gamma^{>}_{\mathcal{N}}\tilde{f}+\mathrm{H.c.} \tag{81}$$

It is worth mentioning that in the real-time evolution the rotating frame frequency μ is still an adjustable parameter and not necessarily synonymous with the chemical potential.

First, let us concentrate on the equation for the mean-field amplitude α. From Eq. (80), we can see that the mean-field evolution consists of two distinct parts: a Hermitian, number-conserving contribution $\Pi_{\mathcal{N}}$, and a part that accounts for condensate number changing collisions out of and into the noncondensate, i.e., $\Upsilon^{<}_{\mathcal{N}}-\Upsilon^{>}_{\mathcal{N}}$. In stationarity, both processes have to vanish identically

$$0=(H^{(0)}+1U_{f^{(c)}}+2U_{\tilde{f}}-\mu)\alpha, \tag{82}$$

$$0=(\Gamma^{\tilde{}\tilde{}}_{\tilde{f}\tilde{f}(1+\tilde{f})}-\Gamma_{(1+\tilde{f})(1+\tilde{f})\tilde{f}})\alpha. \tag{83}$$

Given the constraint on the condensate particle number, it is, in principle, straightforward to solve the Hermitian eigenvalue problem of Eq. (82) and obtain an eigenvalue μ. The later equation Eq. (83) poses a much more challenging constraint on the coupled system. In order to maintain a stationary state, the mean-field has to be ''orthogonal'' to all number changing processes. This means that the normal fluctuations have to adjust self-consistently with respect to the condensate wave function. It is interesting to note that the solutions of this system are infinitely degenerate with respect to a global phase rotation. In other words, the condensate's phase is not pinned down by any restoring force and is free to drift, consequently. However, the later, vector-valued condition of Eq. (83) is satisfied identically if

$$\begin{aligned}0=&\phi^{4''12''1''}\phi^{1''2''3''4''}\delta_{\eta}(\varepsilon_{1''}+\varepsilon_{2''}-\mu-\varepsilon_{4''})\\&\times(1+\tilde{f}_{\varepsilon_{1''}})(1+\tilde{f}_{\varepsilon_{2''}})\alpha_{3''}(1+\tilde{f}_{\varepsilon_{4''}})\\&\times\left[\frac{\tilde{f}_{\varepsilon_{1''}}}{(1+\tilde{f}_{\varepsilon_{1''}})}\frac{\tilde{f}_{\varepsilon_{2''}}}{(1+\tilde{f}_{\varepsilon_{2''}})}-\frac{\tilde{f}_{\varepsilon_{4''}}}{(1+\tilde{f}_{\varepsilon_{4''}})}\right],\end{aligned} \tag{84}$$

vanishes for all components 1. Provided that energy conservation is satisfied exactly, i.e., $\varepsilon_{1''}+\varepsilon_{2''}=\mu+\varepsilon_{4''}$, it is straightforward to verify that a canonical Bose-Einstein distribution

$$\tilde{f}_{\varepsilon}=\frac{1}{e^{\beta(\varepsilon-\mu)}-1}, \tag{85}$$

with an inverse temperature β, is the equilibrium solution. In addition to this functional form of the distribution that is dictated by detailed balance, it is required that all of the excitation energies are above the condensate energy, i.e., $\varepsilon_1>\mu$. Thus the eigenenergy spectrum exhibits a finite gap. From Fig. 5 it can be seen that both the positive energy spectrum of the HFB operator Σ as well as the eigenenergies of $\Sigma_{\mathcal{N}}$, are suitable candidates within this approximation.

Second, the generalized Boltzmann equation, Eq. (81), is stationary if

$$\begin{aligned}0=&(\Gamma^{\tilde{}\tilde{}}_{\tilde{f}\tilde{f}(1+\tilde{f})}+2\Gamma_{f^{(c)}\tilde{f}(1+\tilde{f})}+\Gamma^{\tilde{}\tilde{}}_{\tilde{f}\tilde{f}f^{(c)}})(1+\tilde{f})\\&-(\Gamma_{(1+\tilde{f})(1+\tilde{f})\tilde{f}}+2\Gamma_{f^{(c)}(1+\tilde{f})\tilde{f}}+\Gamma_{(1+\tilde{f})(1+\tilde{f})f^{(c)}})\tilde{f}.\end{aligned} \tag{86}$$

Within the ergodic approximation, the Hermitian part is satisfied identically. On the other hand, there are two distinct types of collisional relaxation processes in Eq. (86). There are the number-conserving in and out rates of the conventional quantum-Boltzmann equation, i.e., $\Gamma^{\tilde{}\tilde{}}_{\tilde{f}\tilde{f}(1+\tilde{f})}(1+\tilde{f})-\Gamma_{(1+\tilde{f})(1+\tilde{f})\tilde{f}}\tilde{f}$. Obviously, both rates match identically under the detailed balance conditions of Eq. (85)

$$\begin{aligned}0=&\phi^{4''12''1''}\phi^{1''2''24''}\delta_{\eta}(\varepsilon_{1''}+\varepsilon_{2''}-\varepsilon_{4''}-\varepsilon_{2})\\&\times(1+\tilde{f}_{\varepsilon_{1''}})(1+\tilde{f}_{\varepsilon_{2''}})(1+\tilde{f}_{\varepsilon_{4''}})(1+\tilde{f}_{\varepsilon_{2}})\\&\times\left[\frac{\tilde{f}_{\varepsilon_{1''}}}{(1+\tilde{f}_{\varepsilon_{1''}})}\frac{\tilde{f}_{\varepsilon_{2''}}}{(1+\tilde{f}_{\varepsilon_{2''}})}-\frac{\tilde{f}_{\varepsilon_{4''}}}{(1+\tilde{f}_{\varepsilon_{4''}})}\frac{\tilde{f}_{\varepsilon_{2}}}{(1+\tilde{f}_{\varepsilon_{2}})}\right].\end{aligned} \tag{87}$$

Both of the two remaining distinct processes in Eq. (86), i.e., $2\Gamma_{f^{(c)}\tilde{f}(1+\tilde{f})}(1+\tilde{f})-2\Gamma_{f^{(c)}(1+\tilde{f})\tilde{f}}\tilde{f}$, as well as the process $\Gamma^{\tilde{}\tilde{}}_{\tilde{f}\tilde{f}f^{(c)}}(1+\tilde{f})-\Gamma_{(1+\tilde{f})(1+\tilde{f})f^{(c)}}\tilde{f}$, involve a condensate particle in the precollision or post-collision channels. Thus, real particles will be transfered between the condensate and the noncondensate, until the rates are balanced. Analogous to the arguments that lead to Eq. (84), it can be shown that a canonical Bose-Einstein distribution is attained in equilibrium.

VI. CONCLUSIONS AND OUTLOOK

In this paper, we have studied aspects of the reversible and irreversible evolution of a condensed atomic gas immersed in the noncondensate. By specializing the kinetic equations [31] for a simple isotropic model, we were able to analyze the equilibrium solution, as well as the dynamic non-equilibrium behavior numerically. In particular, we obtained the excitation spectra of a finite-temperature equilibrium. Moreover, we demonstrated the reversibility of the time-dependent HFB equations far from equilibrium and in the collisionless regime. This is tantamount to noting that the instantaneous occupation numbers of the HFB modes are constants of motion. Finally, we studied the collisional regime for an ergodic distribution of quasiparticles and showed that detailed balance is obtained in the full quantum kinetic theory with a self-consistent canonical Bose-Einstein distribution.

Based on this isotropic model, we can also obtain the collision rates that lead to a self-consistent equilibrium. However, such an analysis is still work in progress and results will be presented in future publications.

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APPENDIX A: CANONICAL TRANSFORMATIONS

A canonical transformation is an inhomogeneous linear combination of creation and destruction operators that preserves the commutation relation [16]. In particular, if $\hat{a}$ and $\hat{a}^\dagger$ denotes a pair of Hermitian conjugated bosonic operators, such that

$$[\hat{a}_1,\hat{a}_2^\dagger]=\delta_{1,2}, \tag{A1}$$

then any affine linear transformation defines a new set of operators b and $\overline{b}$ by

$$\begin{pmatrix} b \\ \overline{b} \end{pmatrix} = T\begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} + d. \tag{A2}$$

In an n-dimensional vector space, T represents a $(2n\times 2n)$ dimensional matrix and d is a $(2n)$-dimensional vector. Such a transformation is canonical if the new pair of operators also satisfies the commutation relation:

$$[b_1,\overline{b_2}]=\delta_{1,2}. \tag{A3}$$

More specifically, the transformation is unitary canonical if the new operators are Hermitian conjugate pairs, i.e., $\overline{b}=b^\dagger$. By inserting Eq. (A2) into Eq. (A3), one finds that the transformation matrices are a representation of the symplectic group $Sp(2n)$:

$$T\sigma_3 T^\dagger=\sigma_3. \tag{A4}$$

In addition, it can be shown that $T^*=\sigma_1 T\sigma_1$ and $T^{-1}=\sigma_3 T^\dagger\sigma_3$. Here, we have introduced the $(2n)$-dimensional Pauli matrices σ_1 and σ_3 as

$$\sigma_1=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\quad \sigma_3=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{A5}$$

APPENDIX B: CAUCHY-SCHWARTZ INEQUALITY

For a positive semidefinite density operator σ and a general operator $\hat{L}$ it follows that the expectation value

$$\langle \hat{L}\hat{L}^\dagger\rangle = \mathrm{Tr}\{\sigma\hat{L}\hat{L}^\dagger\}\geqslant 0 \tag{B1}$$

is never negative. Consequently, the covariance matrix $G^>$ of Eq. (24) must be positive semidefinite $u^\dagger G^> u\geqslant 0$, as well. This can be easily seen, by considering a linear combination of two arbitrary operators $\hat{A}$ and $\hat{B}$, i.e., $L=\alpha\hat{A}+\beta\hat{B}$. By minimizing the positive expression Eq. (B1), one obtains the Cauchy-Schwartz inequality as

$$\langle \hat{A}\hat{A}^\dagger\rangle\langle \hat{B}\hat{B}^\dagger\rangle \geqslant \langle \hat{B}\hat{A}^\dagger\rangle\langle \hat{A}\hat{B}^\dagger\rangle. \tag{B2}$$

In particular, for the special choice of $\hat{A}=\hat{a}_1-\alpha_1$ and $\hat{B}=\hat{a}_2^\dagger-\alpha_2^*$, this implies that the magnitude of the anomalous fluctuations is limited by

$$(1+\tilde{f}_{11})\tilde{f}_{22}\geqslant|\tilde{m}_{12}|^2. \tag{B3}$$

[1] M. H. Anderson *et al.*, Science **269**, 198 (1995).
[2] K. B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995).
[3] C. C. Bradley, C. A. Sackett, and R. G. Hulet, Phys. Rev. Lett. **78**, 985 (1997).
[4] D. G. Fried *et al.*, Phys. Rev. Lett. **81**, 3811 (1998).
[5] S. L. Cornish *et al.*, Phys. Rev. Lett. **85**, 1795 (2000).
[6] B. D. Esry and C. H. Greene, Nature (London) **392**, 434 (1998).
[7] J. Williams *et al.*, Phys. Rev. A **59**, R31 (1999).
[8] J. Williams and M. Holland, Nature (London) **401**, 568 (1999).
[9] M. Matthews *et al.*, Phys. Rev. Lett. **83**, 2498 (1999).
[10] J. Williams *et al.*, Phys. Rev. A **61**, 033612 (2000).
[11] http://amo.phy.gasou.edu/bec.html.
[12] W. Ketterle, D. Durfee, and D. Stamper-Kurn, in *Proceedings of the International School of Physics ''Enrico Fermi,'' Course CXL*, Soc. Italiana di Fisica, Bologna, Italy, edited by M. Inguscio, S. Stringari, and C. Wieman (IOS, Amsterdam, 1999).
[13] B. DeMarco and D. Jin, Science **285**, 1703 (1999).
[14] A. I. Akhiezer and S. V. Peletminskii, *Methods of Statistical Physics* (Pergamon, Oxford, England, 1981).
[15] L. Kadanoff and G. Baym, *Quantum Statistical Mechanics*, Frontiers in Physics (Benjamin, New York, 1962).
[16] J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge, Massachusetts, 1986).
[17] P. Nozières and D. Pines, *The Theory of Quantum Liquids: Superfluid Bose Liquids* (Addison-Wesley, New York, 1990), Vol. II.
[18] A. Griffin, D. W. Snoke, and S. Stringari, *Bose-Einstein Condensation* (Cambridge University Press, Cambridge, England, 1995).
[19] D. Zubarev, V. Morozov, and G. Röpke, *Statistical Mechanics of Nonequilibrium Processes* (Akademie Verlag, Berlin, 1997), Vol. 1, Basic Concepts, Kinetic Theory.
[20] S. Beliaev, Zh. Eksp. Teor. Fiz. **34**, 198 (1958) [Sov. Phys. JETP **34**, 289 (1958)].
[21] J. Kane and L. Kadanoff, J. Math. Phys. **6**, 1902 (1965).
[22] P. Hohenberg and P. Martin, Ann. Phys. (N.Y.) **34**, 291 (1965).
[23] T. R. Kirkpatrick and J. R. Dorfman, J. Low Temp. Phys. **58**, 399 (1985).
[24] N. Proukakis and K. Burnett, Phys. Rev. A **57**, 1230 (1998), and references therein.
[25] C. W. Gardiner and P. Zoller, Phys. Rev. A **61**, 033601 (2000), and references therein.
[26] P. O. Fedichev and G. V. Shlyapnikov, Phys. Rev. A **58**, 3146 (1998).
[27] S. A. Morgan, e-print cond-mat/9911278.
[28] H. T. C. Stoof, J. Low Temp. Phys. **114**, 11 (1999).
[29] E. Zaremba, T. Nikuni, and A. Griffin, J. Low Temp. Phys. **116**, 277 (1999).
[30] F. Dalfovo, S. Giorgini, L. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).

[31] R. Walser, J. Williams, J. Cooper, and M. Holland, Phys. Rev. A **59**, 3878 (1999).
[32] A. J. Moerdijk and B. J. Verhaar, Phys. Rev. Lett. **73**, 518 (1994).
[33] N. R. Newbury, C. J. Myatt, and C. E. Wieman, Phys. Rev. A **51**, R2680 (1995).
[34] P. S. Julienne, F. H. Mies, E. Tiesinga, and C. J. Williams, Phys. Rev. Lett. **78**, 1880 (1997).
[35] K. Huang, *Statistical Mechanics* (Wiley, New York, 1965).
[36] J. Wachter, J. Cooper, M. Holland, and R. Walser (unpublished).
[37] A. Griffin, Phys. Rev. B **53**, 9341 (1996).
[38] M. Lewenstein and L. You, Phys. Rev. Lett. **77**, 3489 (1996).
[39] L. You, W. Houston, M. Lewenstein, and M. Marinescu, Acta Phys. Pol. A **93**, 211 (1998).
[40] Y. Castin and R. Dum, Phys. Rev. A **57**, 3008 (1998).
[41] M. Imamovic-Tomasovica and A. Griffin, http://xxx.lanl.gov/abs./cond-mat/9911402
[42] A. Omont, Prog. Quantum Electron. **5**, 69 (1977).
[43] L. C. Biedenharn and J. D. Louck, *Angular Momentum in Quantum Physics*, Vol. 8 of *Encyclopedia of Mathematics and Its Applications* (Addison-Wesley, Reading, MA, 1981).
[44] D. W. Hutchinson, R. J. Dodd, and K. Burnett, Phys. Rev. Lett. **81**, 2198 (1998).
[45] D. S. Jin *et al.*, Phys. Rev. Lett. **78**, 764 (1997).
[46] S. Stringari, Phys. Rev. Lett. **77**, 2360 (1996).
[47] A. Minguzzi, S. Conti, and M. P. Tosi, J. Phys.: Condens. Matter **9**, L33 (1997).
[48] A. Csordás, R. Graham, and P. Szépfalusy, Phys. Rev. A **57**, 4669 (1998).
[49] M. Naraschewski and R. J. Glauber, Phys. Rev. A **59**, 4595 (1999).
[50] B. Esry, Ph.D. thesis, University of Colorado, 1997 (unpublished).
[51] C. de Boor, *A Practical Guide to Splines* (Springer, Berlin, 1978).
[52] C. de Boor, PPPACK, http://www.netlib.org.
[53] E. Anderson *et al.*, LAPACK, http://www.netlib.org.