Nonequilibrium States of a Quenched Bose Gas

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Yin and Radzihovsky [1] recently developed a self-consistent extension of a Bogoliubov theory, in which the condensate number density \( n_c \) is treated as a mean field that changes with time, in order to analyze a JILA experiment by Makotyn et al. [2] on a \(^{85}\text{Rb} \) Bose gas following a deep quench to a large scattering length. We apply this theory to construct a set of closed equations that highlight the role of \( \dot{n}_c \), which is to induce an effective interaction between quasiparticles. We show analytically that such a system supports a steady state characterized by a constant condensate density and a steady but periodically changing momentum distribution, whose time average is described exactly by the generalized Gibbs ensemble. We discuss how the \( \dot{n}_c \)-induced effective interaction, which cannot be ignored on the grounds of the adiabatic approximation for modes near the gapless Goldstone mode, can affect experimentally measurable quantities such as Tan’s contact.

The recent explosive interest in using ultracold atomic gases as an excellent platform for studying the dynamics of strongly correlated systems driven out-of-equilibrium by slow (adiabatic) or sudden (quenched) changes to system parameters [3–5] has been fueled by the unprecedented ability to tune such system parameters, in particular the interatomic interaction [6], and early experimental [7–10] and theoretical [11–17] explorations of nonequilibrium dynamics. At the forefront of such studies are questions regarding nonequilibrium states reached after quenching [4], whose observation hinges on the ability of many-body systems to maintain coherence on time scales much longer than the equilibration time of the particles in the systems. The main obstacle preventing cold toms, especially those with a large scattering length \( a \), from acquiring such a long coherence time is three-body recombination, in which two atoms in a trap form a diatomic molecule with a third atom escaping from the trap, causing losses. This poses less of a challenge in fermionic systems, thanks to the Pauli exclusion principle which tends to suppress three-body recombination [18]. As such, in Fermi gases tuned across or close to the Feshbach resonance, where \( a \) goes to infinity, researchers have observed, among other things, the crossover from Fermi to Bose superfluids [19–21], rich phase separation scenarios [22], and universalities of Fermi gases [23–27].

By contrast, we are less fortunate with bosonic systems. In the weak interaction limit, the three-body loss rate \( \propto n^2 a^4 \) [28] increases with \( a \) (\( > 0 \)) far faster than the equilibration rate \( \propto n a^2 v \), where \( n \) is the atom number density and \( v \) is the average velocity. In the strong interaction limit, systems are highly nonlinear. In the extreme case of unitarity, where \( a \to \infty \), the interatomic distance, \( n^{-1/3} \), remains the only physically relevant length scale, and the unitary Bose gas [29–34] is expected to display universal properties akin to those of a Fermi gas at unitarity [35–37]. This means, on purely dimensional grounds, that both rates will be of the same order of magnitude as the Fermi energy \( \epsilon_F = \hbar^2 k_F^2/2m \), where \( k_F = (6\pi^2 n)^{1/3} \) is the Fermi momentum. It was unclear which one dominates until recently when a JILA experiment on \(^{85}\text{Rb} \) by Makotyn et al. [2] firmly established that the three-body loss rate is much slower than the equilibration rate. This pleasant surprise opens the door to the possibility of exploring the rich physics underlying strongly interacting Bose gases [29–34] through quenched nonequilibrium dynamics [1, 38].

Of particular relevance here is a theoretical analysis of the JILA experiment by Yin and Radzihovsky [1] who, in the spirit of Bogoliubov mean-field theory, divided the Bose gas at zero temperature into a quantum system of Bogoliubov quasiparticles and a condensate of number density \( n_c \), which is treated as a dynamical mean field (as opposed to a fixed constant as done by Natu and Mueller [39]). We explore this same topic using this same approach. In order to distinguish as well as highlight our work, we point out an important feature inherent to any Bogoliubov inspired mean-field theories: mean fields \( n_c \) here), which act like control (albeit self-generated) parameters to the quantum system describing quasiparticles, change with time even after quenching. This may be contrasted with many existing models, particularly those in one dimension (1D) to which powerful techniques such as bosonization are accessible [5], where the control parameters, after quenching, are all fixed independent of time.

Motivated by this, we derive a set of closed equations (9) and (13), which depend explicitly not only on \( n_c \) but also on \( \dot{n}_c \), thereby allowing us to identify that the role of \( \dot{n}_c \) is to induce between quasiparticles an effective interaction proportional to \( \dot{n}_c \). Will such a system reach a steady state? The answer seems affirmative from both the measurement in experiment [2] and the numerical investigation in theory [1]. Here, we show analytically that this is true in the thermodynamic limit. What are the properties of such a steady state? This stationary state is characterized by a time-independent condensate density and a steady but periodically changing momentum
distribution of quasiparticles. The authors of the recent JILA experiment [2], while recognizing the excellent fit between measured momentum and an ideal Bose gas distribution, were nevertheless open to other possibilities. We show analytically that the time average of this distribution is described exactly by the generalized Gibbs ensemble. We stress that our formalism, where the role of \( \hat{n}_c \) is explicitly built in, lends itself naturally to the adiabatic theorem, allowing us to estimate straightforwardly the effect of the \( \hat{n}_c \)-induced interaction on system dynamics.

We model the interacting Bose gas (with a broad Feshbach resonance) by a single-channel grand-canonical Hamiltonian,

\[
\hat{H} = \int d^3r \hat{\psi}^\dagger(r) \hat{\psi}(r) + \frac{g}{2} \int d^3r \hat{\psi}^\dagger(r) \hat{\psi}^2(r),
\]

where \( \hat{\psi}(r) \) is the bosonic field operator in position space, \( \hat{\psi}_0 = -\hbar^2 \nabla^2/2m - \mu \) is the single-particle Hamiltonian operator with \( \mu \) the chemical potential, and \( g = 4\pi\hbar^2a/m \) measures the contact interaction. The dynamics of such a system following a sudden quench where \( a(g) \) changes abruptly from \( a_i \) \((g_i)\) to \( a_f \) \((g_f)\) can, in general, be quite complicated. As a simplification, we assume that the system remains, throughout its evolution, in a state where the Bogoliubov perturbative ansatz, \( \hat{\psi}(r) = \hat{\psi} + \hat{\delta}\hat{\psi}(r) \), remains valid. Here, as in equilibrium problems, \( \hat{\delta}\hat{\psi}(r) = \sum_{k \neq 0} \hat{a}_k e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V} \) with \( V \) the total volume, is an operator describing fluctuations around the macroscopic (but uniform) condensate of density \( n_c = |\hat{\psi}|^2 \) and chemical potential \( \mu = gn_c \). Following Ref. [1], we treat \( n_c \) as a dynamical mean field, \( n_c(t) \). The Hamiltonian after quenching \((t > 0^+)\), up to second order in \( \hat{a}_k \), then reads

\[
\dot{\hat{H}} = \sum_{k \neq 0} \left( e_k + g f n_c \right) \hat{a}_k^\dagger \hat{a}_k + \frac{g f n_c}{2} \left( \hat{a}_k^\dagger \hat{a}_k^\dagger - \hat{a}_k \hat{a}_k \right),
\]

(2)

with \( e_k = \hbar^2 k^2/2m \) the kinetic energy of an atom. Note that the same \( \dot{\hat{H}} \), with \( g f \) replaced with \( g_i \), describes a system in equilibrium before quenching \((t < 0^-)\). A quadratic Hamiltonian like Eq. (2) can be diagonalized into

\[
\hat{H} = H_0 + \sum_{k \neq 0} E_k(t) \hat{\gamma}_k^\dagger(t) \hat{\gamma}_k(t) \quad \text{[with]} \quad H_0 = -Vg f n_c^2/2 + \frac{1}{2} \sum_{k \neq 0} \left( E_k - e_k - g f n_c \right) \]

(3)

by means of a Bogoliubov transformation,

\[
\begin{bmatrix}
\hat{a}_k \\
\hat{\gamma}_k^\dagger \\
\hat{a}^\dagger_{-k} \\
\hat{\gamma}_{-k}^\dagger
\end{bmatrix} = \begin{bmatrix}
\hat{u}_k & \hat{v}_k & 0 & 0 \\
\hat{v}^*_k & \hat{u}_k & 0 & 0 \\
0 & 0 & \hat{u}_k & \hat{v}_k \\
0 & 0 & \hat{v}^*_k & \hat{u}_k \\
\end{bmatrix} \begin{bmatrix}
\hat{\gamma}_k \\
\hat{\gamma}_{-k}^\dagger \\
\hat{\gamma}_{-k}^\dagger \\
\hat{\gamma}_k \\
\end{bmatrix},
\]

(4)

where

\[
\begin{align*}
\hat{u}_k(t) & = \sqrt{\frac{1}{2} \left( \frac{e_k + g f n_c(t)}{E_k(t)} \pm 1 \right)}, \\
\hat{v}_k(t) & = \sqrt{\frac{1}{2} \left( \frac{e_k + g f n_c(t)}{E_k(t)} \mp 1 \right)},
\end{align*}
\]

(5)

are the Bogoliubov parameters and

\[
E_k(t) = \sqrt{e_k(e_k + 2g f n_c(t))},
\]

(6)

is the quasi-particle energy dispersion. The time evolution of the system is governed by the Heisenberg equation of motion for operator \( \hat{\gamma}_k \),

\[
\frac{d\hat{\gamma}_k}{dt} = -\frac{i}{\hbar} \left[ \hat{\gamma}_k, \hat{H}_2 \right] + \frac{\hbar^2}{2E_k(t)} \hat{\gamma}_k^\dagger \hat{\gamma}_k,
\]

(7)

where we have taken into consideration that the operator \( \hat{\gamma}_k \) defined in Eq. (3), depends explicitly on time via \( n_c(t) \). Applying the Bogoliubov transformation in Eq. (3), we change Eq. (6) into

\[
\frac{d\hat{\gamma}_k}{dt} = -\frac{i}{\hbar} E_k(t) \hat{\gamma}_k + g f n_c(t) \frac{\epsilon_k}{2E_k^2(t)} \hat{\gamma}_k^\dagger \hat{\gamma}_k.
\]

From the final term in Eq. (7), which would have been absent had we ignored the partial derivative in Eq. (6), we see that \( \hat{n}_c(t) \neq 0 \) is to induce between quasiparticles an effective interaction \( g f n_c(t) \epsilon_k/2E_k^2(t) \). It is as if the quasiparticles were subject to a time-varying control parameter. We now change the dynamical variables from operators, \( \hat{\gamma}_k(t) \) and \( \hat{\gamma}_{-k}^\dagger(t) \), to complex numbers, \( c_k(t) \) and \( d_k(t) \), via the transformation

\[
\begin{bmatrix}
\hat{\gamma}_k(t) \\
\hat{\gamma}_{-k}^\dagger(t)
\end{bmatrix} = \begin{bmatrix}
\hat{c}_k(t) & -\frac{\hbar}{\epsilon_k} \hat{d}_k(t) \\
\frac{\hbar}{\epsilon_k} \hat{d}^*_k(t) & \hat{c}_k^\dagger(t)
\end{bmatrix} \begin{bmatrix}
\hat{\gamma}_k \\
\hat{\gamma}_{-k}^\dagger
\end{bmatrix}
\]

(8)

where \( |c_k(t)|^2 - |d_k(t)|^2 = 1 \) and \( \hat{c}_k \) is the quasi-particle operator defined with respect to the pre-quench vacuum \( |0^-\rangle \). \( \hat{\gamma}_k(t) \) thus defined is a solution to Eq. (7) provided that

\[
\frac{d}{dt} \begin{bmatrix}
\hat{c}_k \\
\hat{d}_k
\end{bmatrix} = \begin{bmatrix}
-\frac{i}{\hbar} E_k(t) & -\frac{\epsilon_k g f n_c(t)}{2E_k^2(t)} \\
-\frac{\epsilon_k g f n_c(t)}{2E_k^2(t)} & +\frac{i}{\hbar} E_k(t)
\end{bmatrix} \begin{bmatrix}
\hat{c}_k \\
\hat{d}_k
\end{bmatrix},
\]

(9)

where \( \hat{c}_k \) and \( \hat{d}_k \) are subject to the initial condition

\[
c_k(0^+) = u^*_k u_k - v^*_k v_k, \quad d_k(0^+) = u^*_k v_k - v^*_k u_k.
\]

(10)

In a quench experiment where the quench parameter is changed from an initial to a final value very rapidly, specifically in a time much shorter than any other characteristic time scale of the system, one can apply the so-called sudden approximation in which the state of the system immediately after quenching at \( t = 0^+ \) is assumed to be the same as that immediately before quenching, namely, \( \hat{a}_k(0^-) = \hat{a}_k(0^+) \) and \( n_c(0^-) = n_c(0^+) \). The initial condition in Eq. (10) is derived from this sudden approximation, where \( u_k, v_k, \) and \( E_k(u_k^+, v_k^+), E_k^c(u_k^-, v_k^-) \) are the same as Eqs. (4) and (5) except that \( g_f \) and \( n_c \) are set to their \( t = 0^- \) \((t = 0^+) \) values.

The condensate density \( n_c(t) \) in Eq. (9) is to be obtained self-consistently from total particle number conservation, \( n_c(t) = n - \sum_k n_k(t) \), where \( n_k(t) \) is set to \( t = 0^- \) \((t = 0^+) \) values.

The condensate density \( n_c(t) \) in Eq. (9) is to be obtained self-consistently from total particle number conservation, \( n_c(t) = n - V^{-1} \sum_k n_k(t) \), where \( n_k(t) \) is set to \( t = 0^- \) \((t = 0^+) \) values.
is the momentum distribution of quasiparticles (or non-condensed particles). (Throughout, averages like $\langle \hat{A} \rangle$ will always be defined with respect to the pre-quench vacuum: $\langle 0^- | \hat{A} | 0^- \rangle$.) From the time derivative of the number equation, it follows that
\[
\frac{dn_c(t)}{dt} = -g_f n_c \frac{1}{V} \sum_{k \neq 0} \left\{ D_k - \frac{2}{\hbar} \text{Im} [c_k^* d_k] \right\},
\]
where
\[
D_k = 2 \left( v_k - \frac{u_k \epsilon_k}{2E_k^*} \right) [v_k |c_k|^2 + u_k \text{Re} (c_k^* d_k)] + (v_k \leftrightarrow u_k, c_k \leftrightarrow d_k).
\]
Finally, with the help of Eqs. (4), we arrive at
\[
\frac{dn_c(t)}{dt} = 2g_f n_c \frac{1}{V} \sum_{k \neq 0} \text{Im} [c_k^* (t) d_k(t)],
\]
which, together with Eq. (9), forms a closed set of equations. In what follows, we use Eqs. (9) and (13) to study the quenched dynamics.

First, we show self-consistently that in the limit $t \to \infty$, such a set of equations support a steady-state characterized by $\dot{n}_c(t) \approx 0$ or $n_c(t) \approx n_c^\ast$, a variable with superscript $\ast$ denotes the steady state value. The proof begins with the assumption that $\dot{n}_c(t) \approx 0$, which then leads, from Eq. (9), to $c_k(t) \approx c_k^\ast \exp (-\frac{1}{\hbar} E_k^* t)$ and $d_k(t) \approx d_k^\ast \exp (\frac{1}{\hbar} E_k^* t)$, where $E_k^*$ is Eq. (5) when $n_c$ is replaced with $n_c^\ast$. To check the self-consistency, we substitute these long time $c_k(t)$ and $d_k(t)$ into Eq. (13), which results in $\dot{n}_c(t) \propto \frac{1}{V} \sum_{k \neq 0} \text{Im} [c_k^* d_k^\ast \exp (i 2E_k^* t/\hbar)].$ For a finite system, $E_k^*$ belongs to a finite discrete set and the sum will lead to a time evolution reminiscent of the collapse and revival of Rabi oscillations. But, in the thermodynamic limit where $V \to \infty$, $E_k^*$ is continuous in $k$ and the discrete sum is transformed into an integral $\dot{n}_c(t) \propto \frac{1}{\hbar} \int \text{Im} [c_k^* d_k^\ast \exp (i 2E_k^* t/\hbar)] $ dk, this integral, due to the destructive interference, vanishes in the limit $t \to \infty$ for any well-behaved $k^2 c_k^* d_k^\ast$. Thus, we conclude that a steady-state with $\dot{n}_c \approx 0$ exists in the thermodynamic limit. Note that in this steady state, $n_k(t)$ displays persistent oscillations in time with the momentum-dependent frequency $E_k^*/\hbar$, but this lack of decoherence is expected within the collisionless Bogoliubov approximation (as is the case in this study) where real “collisions” between the Bogoliubov quasi-particles are absent.

How might we characterize the asymptotic steady-state momentum distribution, $n_k(t)$, reached after quench? For an isolated integral system, Rigol et al. [16], motivated by a seminal experiment by Kinoshita et al. [10], suggested that the steady state be described by the generalized Gibbs ensemble, which maximizes the many-body von-Neumann entropy, subject to constraints imposed by all integrals of motion, rather than described by the standard thermal ensemble, which has only a handful of integrals of motion, such as total energy, total particle number, etc. This conjecture is confirmed both numerically [16] and analytically [17] for some correlation functions in 1-D quantum systems [5]. The present model is different since it consists of two parts: condensate and quasiparticles. As the two parts interact with each other, the quasiparticle system is, by itself, not closed, and quantities such as $\hat{\gamma}_k^\dagger \hat{\gamma}_k$ are time-dependent. However, in the limit $t \to \infty$, the $\hat{\gamma}_k^\dagger \hat{\gamma}_k$ become (approximately) constants of motion, and the quasiparticle system can be regarded as an integral system where the degrees of freedom are equal in number to the integrals of motion.

We now show analytically that the time average of $n_k(t)$ at steady state follows exactly the generalized Gibbs ensemble described by the density operator $\hat{\rho}_G = Z_{G}^{-1} \exp (-\sum_k \beta_k \hat{\gamma}_k^\dagger \hat{\gamma}_k)$, where $Z_G = \text{Tr} \exp (-\sum_k \beta_k \hat{E}_k \hat{\gamma}_k^\dagger \hat{\gamma}_k)$ is the partition function. In the Gibbs ensemble, there corresponds to each mode $k$ an (inverse) temperature $\beta_k$, determined by
\[
\langle \hat{\gamma}_k^\dagger \hat{\gamma}_k \rangle_G \equiv \text{Tr} \left( \hat{\gamma}_k^\dagger \hat{\gamma}_k \hat{\rho}_G \right).
\]
This may be contrasted with the standard thermal ensemble, which is described by a unique temperature $\beta$ independent of momentum. A straightforward application of Eq. (3) yields a momentum distribution, $n_k(t) = \langle \hat{a}_k^\dagger (t) \hat{a}_k (t) \rangle$, in the form of
\[
n_k(t) = (u_k^2 + v_k^2) \langle \hat{\gamma}_k^\dagger (t) \hat{\gamma}_k (t) \rangle + v_k^2 - u_k v_k \langle \hat{\gamma}_k^\dagger (t) \hat{\gamma}_{-k} (t) + \hat{\gamma}_{-k}^\dagger (t) \hat{\gamma}_k (t) \rangle,
\]
on one hand, and a momentum distribution in the Gibbs ensemble, $n_k(t)_G = \langle \hat{a}_k^\dagger (t) \hat{a}_k (t) \rangle_G$, in the form of
\[
n_k(t)_G = (u_k^2 + v_k^2) \langle \hat{\gamma}_k^\dagger (t) \hat{\gamma}_k (t) \rangle_G + v_k^2,
\]
on the other hand. By virtue of the identity in Eq. (14), the two distributions are the same apart from the second line of Eq. (15). However, in the limit $t \to \infty$, using Eq. (8) and $c_k(t) \approx c_k^\ast \exp [-i E_k^* t/\hbar]$, and $d_k(t) \approx d_k^\ast \exp (i E_k^* t/\hbar)$, one can find that this second line equals $2u_k v_k \text{Re} (c_k^* d_k^\ast \exp [-i E_k^* t])$, which is a periodic function of time and thus averages to zero. This concludes the proof that the time average of $n_k(t)$ at steady state is fitted exactly by the generalized Gibbs ensemble distribution. A comparison given in Fig. 1 indicates that this nonequilibrium distribution (solid curve) is different from the equilibrium one (dashed curve).

The distribution at large momenta is of particular interest as it is related to Tan’s contact [40] which is one of the universal properties of a quantum gas irrespective of its quantum statistics. By solving Eqs. (9) and (11) under the condition that $\dot{n}_c(t)$ be zero, we arrive at the results of Ref. [1], which consists of a distribution, $n_k(t) = n_{k,1}(t) + n_{k,2}(t)$, given by
\[
n_{k,1}(t) = \frac{\epsilon_k [\epsilon_k + (g_f + g_v) n_v] \epsilon_k + g_v n_v (t)}{2E_k^* E_k^*} - \frac{1}{2}, \quad (17)
n_{k,2}(t) = -\epsilon_k (g_f - g_v) g_v n_v (t) \cos [2 \phi_k (t)], \quad (18)
\]
It is then straightforward to show that the ratio between the \( \dot{n}_c \)-induced interaction, \( \hbar \varepsilon_k g_f \dot{n}_c(t) / 2E_k^2(t) \), and the quasiparticle energy, \( E_k(t) \),

\[
\eta_k(t) \equiv \frac{\hbar \varepsilon_k g_f |\dot{n}_c(t)|}{2E_k^3(t)},
\]

represents the first-order correction relative to the zeroth order solution. \( \eta_k(t) \) in Eq. (24) can also be used as a nice figure of merit measuring the adiabaticity of the system when \( n_c(t) \) changes with time. Figure 2(b) is a contour plot of \( \eta_k(t) \) using \( n_c(t) \) and \( \dot{n}_c(t) \) obtained from Eq. (20) as the zeroth-order solution. The formation of a Bose condensate is due to the spontaneous breaking of a continuous symmetry, which is always accompanied by a gapless Goldstone mode. This explains why the adiabatic condition tends to break down for modes near the Goldstone mode \( (k = 0) \), particularly during the early stage when \( |\dot{n}_c(t)| \) is still appreciable. Thus, Eqs. (17) and (18) fail to describe the momentum distribution at small momenta. Note that \( n_c(t) \) is a collective variable, whose value depends on the histories of all modes of momenta, be they small or large. As a result, as illustrated in Fig. 2(a), \( n_c(t) \) integrated from Eq. (20), which uses Eqs. (17) and (18) as the small momentum distribution, is noticeably different from \( n_c(t) \) integrated exactly. This can have measurable effects on observables such as Tan’s contact \( C \), which (in the units of \( 16\pi^2 n^{4/3} \)) changes from 0.57 when \( \dot{n}_c(t) \) is included to 0.517 when it is neglected, for the example in Fig. 2(a).

In summary, using a self-consistent extension of a Bogoliubov theory [1] in which the condensate number density \( n_c \) is treated as a time-dependent mean field, we have constructed a set of closed equations that highlight the role of \( \dot{n}_c \), which is to induce an effective interaction between quasiparticles. We have used this set of equations to explore the nonequilibrium dynamics of a Bose gas.
gas that has undergone a deep quench to a large scattering length. We have shown analytically that the system after quenching can reach a steady state in which the time-averaged momentum distribution is described exactly by the generalized Gibbs ensemble. We discussed how the $\dot{n}_c$-induced effective interaction, which cannot be ignored on grounds of adiabatic approximation for modes near the gapless Goldstone mode, can affect the experimentally measurable quantities such as Tan’s contact.

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