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Kinetic model of trapped finite-temperature binary condensates

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We construct a nonequilibrium theory for the dynamics of two interacting finite-temperature atomic Bose-Einstein condensates and use it to numerically estimate the relative rates of the arising collisional processes near equilibrium. The condensates are described by dissipative Gross-Pitaevskii equations, coupled to quantum Boltzmann equations for the thermal atoms. The density-density interactions between atoms in different components facilitate a number of transport processes of relevance to sympathetic cooling: in particular, considering realistic miscible and immiscible trapped atomic $^{87}$Rb-$^{41}$K and $^{87}$Rb-$^{85}$Rb condensate mixtures, we highlight the dominance of an intercomponent scattering process associated with collisional “exchange” of condensed and thermal atoms between the components close to equilibrium.

Introduction. The unprecedented control of trapped neutral cold atom experiments enables the creation and study of degenerate multicomponent systems, including Bose-Bose [1], Bose-Fermi [2], and Fermi-Fermi [3,4] mixtures, and the related problems of spinor gases [5] and artificial gauge fields [6]. In two-component systems, cooling to quantum degeneracy is typically performed through a combination of evaporative [7] and sympathetic [8] cooling techniques. For bosonic mixtures, this leads to condensation in differing hyperfine states of an atom ($^{87}$Rb [1,8–10]), differing isotopes (e.g., $^{87}$Rb-$^{85}$Rb [11], $^{168}$Yb-$^{174}$Yb [12]), or differing elements (e.g., $^{87}$Rb-$^{41}$K [13,14], $^{87}$Rb-$^{133}$Cs [15,16], $^{87}$Rb-$^{84}$Sr and $^{87}$Rb-$^{88}$Sr [17], and $^{87}$Rb-$^{23}$Na [18]). Interest in such systems has focused on understanding numerous properties, including equilibrium profiles [19–23], stability properties [24,25], collective excitations [20,26], vortices [27], solitary waves [28], and dissipative [29] and quenched dynamics [30]; these effects depend critically on the relative interatomic interactions within and between the species, which determine whether the emerging condensates overlap spatially or phase separate [19,20].

The description of bosonic mixtures is typically either focused on the low-temperature (Gross-Pitaevskii) [31] or high-temperature (Boltzmann) limit [32] or on treating the condensate in contact with a static heat bath [33–35]. Alternative approaches are based on classical field methods (which ignore the dynamics of the high-lying thermal modes [30,36]) or on number-conserving methods (which explicitly include only the backaction of the thermal cloud on the condensate [37,38]). Moreover, although related kinetic models have been derived in the context of spinor gases [39,40], there has been to date no critical assessment of the relative importance of the various collisional processes at finite temperatures.

In this work we (i) present a self-consistent model for the study of partly condensed bosonic mixtures in the presence of dynamical condensates and thermal clouds (shown schematically in Fig. 1) and (ii) perform detailed numerical calculations at equilibrium to shed light on the relative importance of those processes for experimentally accessible miscible and immiscible mixtures. A key conclusion is the estimation of the importance of a novel “cross-condensate-exchange” term found to dominate as soon as both species exhibit condensation.

Our approach is a generalization of the Zaremba-Nikuni-Griffin (ZNG) kinetic model [41–43], which, in the context of single-component condensates, has proven extremely useful in describing collective modes [44], condensate growth [45], dynamics of macroscopic excitations [46], and surface evaporative cooling [47]. This approach is based on the decomposition of the Bose field operator into a symmetry-breaking part and its fluctuations and a separation of time scales argument (see also Refs. [48–50]): in our analysis, we explicitly separate slowly evolving variables for the condensate and thermal clouds, whose nonvanishing mean values are defined by appropriate dynamical equations, from those evolving on the more rapid collisional time scales. A careful self-consistent perturbative treatment of the latter in the context of an appropriate perturbing Hamiltonian (details to appear elsewhere) enables

![FIG. 1. (Color online) Schematic representation of the collisional model. The two trapped condensates are denoted (a) (left) and (b) (right). Arrows indicate the various mean-field and collisional transport processes occurring within and between condensates and noncondensates of different components.](image-url)
Coupled kinetic theory. The second-quantized Hamiltonian describing the interacting binary mixture is

\[ \hat{H} = \sum_{j=a, b} \int d\mathbf{r} \hat{\Psi}_j^\dagger \left( \hat{H}_{0, j} + \frac{1}{2} \sum_{k=a, b} g_{kj} \hat{\Psi}_k^\dagger \hat{\Psi}_k \right) \hat{\Psi}_j, \]

where \( \hat{\Psi}_j \equiv \hat{\Psi}_j(\mathbf{r}) \) is the annihilation operator for a species- \( j \) atom, \( \hat{H}_{0, j} = -\hbar^2/(2m_j) \nabla^2 + V_j(\mathbf{r}), \) and \( g_{kj} = 2\pi \hbar^2 a_{kj}/m_j, \) where \( a_{kj} \) is the scattering length between atoms in components \( j \) and \( k. \) \( m_j \) is the reduced mass, \( m_j \) is the mass of a boson in component \( j, \) and \( V_j(\mathbf{r}) \) is the trapping potential.

The condensed and noncondensed components are separated by the Beliaev decomposition \( \hat{\Psi}_j = \phi_j + \delta_j, \) with condensate evolution equations obtained from the Heisenberg equations of motion for \( \phi_j \) as

\[ i\hbar \frac{\partial \phi_j}{\partial t} = \left[ -\frac{\hbar^2}{2m_j} \nabla^2 + U_j \right] \phi_j + g_{kj}[(\delta_j \delta_k) \phi_j + (\delta_k \delta_j) \phi_k + (\delta_j \delta_k) \phi_k], \]

where \( \langle \cdots \rangle \) denotes averages (with \( \langle \delta_j^{(i)} \rangle = 0 \)), \( j, k \in \{a, b\} \) and \( U_j(\mathbf{r}, t) = V_j(\mathbf{r}) + g_{kj}(n_{kj} + 2n_j) + g_{kj}(n_{kek} + n_k) \) is the effective condensate potential. Following established techniques [41], we identify the condensate fields \( \phi_j \) (corresponding condensate densities \( n_{kj} = |\phi_j|^2 \)) and the diagonal noncondensate densities \( n_j = |\delta_j|^2 \) as the only relevant slowly varying quantities of interest. Triplet anomalous averages \( \langle \delta_j \delta_k \delta_{\bar{k}} \rangle \) and \( \langle \delta_j \delta_k \delta_{\bar{k}} \rangle \) are treated perturbatively (via adiabatic elimination [48,49]), giving rise to well-known source terms, and we only maintain energy-conserving contributions, thus also discarding pair anomalous averages \( \langle \delta_j \delta_k \rangle \) and \( \langle \delta_k \delta_j \rangle \) [51]. An important aspect of our work (see also Refs. [36,38]) is that we explicitly maintain perturbative corrections arising from the off-diagonal terms \( \langle \delta_j \delta_k \rangle \). As a result, the equation of motion for component \( j \) takes the form

\[ i\hbar \frac{\partial \delta_j}{\partial t} = \left[ -\frac{\hbar^2}{2m_j} \nabla^2 + U_j - i(R^{jj} + R^{kj} + R^{kj}) \right] \phi_j. \]

It contains a number of source terms:

\[ R^{jj}(\mathbf{r}, t) = -ig_{kj}(\delta_j \delta_k) / \phi_j \]

appearing in Eq. (3) describes the intracomponent scattering of condensate and noncondensate particles and is well-known from single-component ZNG theory [41];

\[ R^{kj}(\mathbf{r}, t) = -ig_{kj}(\delta_j \delta_k) / \phi_j \]

is a direct generalization of \( R^{jj} \) to binary condensates, describing the intercomponent scattering of condensed and noncondensated atoms. \( R^{kj}(\mathbf{r}, t) = -ig_{kj}(\delta_j \delta_k) / \phi_j \)

is qualitatively different from the other two [see Eq. (6) below]. \( R^{kk}, R^{jj}, \) and \( R^{kj} \) are defined through their relation to the collision integrals \( C_{12}^{kj}, C_{12}^{ij}, \) and \( C_{12}^{ij} \) given below.

To construct a self-consistent theory including the evolution of the noncondensate, the multicomponent single-particle Wigner distribution is introduced as

\[ f^{ij}(\mathbf{p}, t) = \int d\mathbf{r} d\mathbf{r}' e^{-i\mathbf{r} \cdot \mathbf{p}} \langle \hat{\Psi}_j^\dagger(\mathbf{r}) \hat{\Psi}_k(\mathbf{r}') \rangle. \]

We restrict our analysis to the diagonal terms of \( f^{ij}(\mathbf{p}, t), \) i.e., \( f^{jj}(\mathbf{p}, t) \equiv f^{jj}(\mathbf{p}_j, t) \), valid in the absence of coherent couplings between states. The kinetic equation for component \( j \) is

\[ \frac{\partial}{\partial t} f^{ij} + \frac{1}{m_j} \mathbf{p} \cdot \nabla f^{ij} - \nabla_p f^{ij} \cdot \mathbf{F}_U^j = (C_{12}^{jj} + C_{12}^{ij} + C_{12}^{ij} + C_{22}^{jj}). \]

The Hartree-Fock potential that noncondensed atoms in component \( j \) feel is

\[ U_j^f(\mathbf{r}, t) = \frac{1}{2} \int d\mathbf{p} / (2\pi \hbar)^3 \int d\mathbf{p}_j \int d\mathbf{p}_k f^{kj(\mathbf{p}_j, \mathbf{r}, t)} U_j^f(\mathbf{p}_j) \]

The various collisional contributions to the kinetic scattering of particles for the \( a \) component are summarized in Fig. 2. Diagrams (i) and (ii) concern collision integrals describing the scattering of condensed and noncondensed particles, while diagrams (iv) and (v) show scattering amongst noncondensed atoms.

The collision integral \( C_{12}^{ij} \) (encapsulating \( C_{12}^{ij} \)) appearing in Eq. (4) is defined by

\[ C_{12}^{ij} = \int d\mathbf{p}_j \int d\mathbf{p}_k \int d\mathbf{p}_4 \times \left[ n_{c,k} \delta(\mathbf{p}_j^k + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4) \delta(\mathbf{p}_j^k + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4) \right]. \]

It describes the scattering of a condensate atom and a noncondensate atom into thermal states, and its inverse process [Figs. 2(ii) and 2(iii)], with the Kronecker delta \( \delta_{kj} \) accounting for enhanced scattering of atoms within the same species (\( C_{12}^{ij} \) subcase). Here \( \varepsilon_{pj}^j = p_j^2 / 2m_j + U_j^f \) is the Hartree-Fock potential.

FIG. 2. (Color online) Each diagram represents a kinetic energy and momentum conserving collision between atoms. Squares and circles represent condensate and thermal atoms, respectively. Component \( a \) particles are solid blue, while \( b \) particles are open red. Diagrams for the \( b \) component are obtained by interchanging the two colors in each square and circle.
energy, $\varepsilon_i = \mu_i + \frac{1}{2}m_i v_{e,i}^2$ defines the condensate energy, and $p_i^c = m_i v_{e,i}$ gives the condensate momentum.

The collision integral $C_{12}^{kj}$ is defined from the average of an off-diagonal pair of fluctuation operators, $\langle \hat{\xi}^j_k \hat{\delta} \rangle (j \neq k)$ (in contrast to all other ZNG source terms originating from triplet terms $\delta^3 \hat{\delta} \hat{\delta}$) [39–41], as

$$C_{12}^{kj} = \frac{2 \pi g_{kj}^2}{\hbar} n_{c,k} n_{c,j} \int dp_1 \int dp_2 \int dp_3 \int dp_4 \times \delta(p_1 + p_2 - p_3 - p_4) \delta(\varepsilon_1^c + \varepsilon_2^c - \varepsilon_3^c - \varepsilon_4^c) \times [(f_1^k + 1) f_2^j f_3^j f_4^j - f_1^k f_2^j (f_3^j + 1) (f_4^j + 1)],$$

(6)

Although physically intuitive, this term is qualitatively different from the collision integral of Eq. (5), as it describes a process [Fig. 2(iii)] whereby one condensate and one noncondensate atom from different components scatter into a thermal state and a condensed state, respectively.

The final collision processes $C_{22}^{kj}$ and $C_{21}^{kj}$ in Eq. (4) describe the scattering between noncondensate atoms of the same ($k = j$) or different ($k \neq j$) species, given by

$$C_{22}^{kj} = (1 + \delta_{kj}) \frac{g_{kj}^2}{(2\pi \hbar)^6} \int dp_2 \int dp_3 \int dp_4 \times \delta(p + p_2 - p_3 - p_4) \delta(\varepsilon_1^c + \varepsilon_2^c - \varepsilon_3^c - \varepsilon_4^c) \times [(f_1^j + 1) f_2^j f_3^j f_4^j - f_1^j f_2^j (f_3^j + 1) (f_4^j + 1)],$$

(7)

### Numerical results.

To gain insight into the relative importance of the collision rates we compute their temperature dependence for experimentally relevant equilibrium $^{87}\text{Rb,}^{41}\text{K}$ and $^{87}\text{Rb,}^{85}\text{Rb}$ mixtures in isotropic harmonic traps ($\omega = 2\pi \times 20 \text{ Hz}$) and a total atom number $N_j = 10^5$ in each component. These mixtures were chosen as their tunable scattering lengths [11,13,14] enable the probing of both miscible $\Lambda = g_{12}/\sqrt{g_{11}g_{22}} < 1$ and immiscible ($\Lambda > 1$) regimes. By re-expressing $C_{12}^{kj} = C_{12}^{kj,\text{out}} - C_{12}^{kj,\text{in}}$ (and analogously for $C_{22}^{kj}$ and $C_{21}^{kj}$), we explicitly identify “in” and “out” scattering rates, which are equal at equilibrium. Following Refs. [41,43], we define collisional rates $C_{12}^{kj}(\omega) = \int dp/(2\pi \hbar)^3 C_{12}^{kj,\text{out}}$ that give the number of atoms leaving a phase-space volume $d\Omega dp/\hbar$ per unit time as a result of collisions, for a perturbation from equilibrium. By transforming to the center-of-mass frames, the collision rates can be written as $C_{12}^{kj}(\omega) = \int dp/(2\pi \hbar)^3 C_{12}^{kj,\text{out}}$. While the $\gamma_{12}^{kj}$ collision scattering rate, $\gamma_{12}^{kj} = \int dp/(2\pi \hbar)^3 C_{12}^{kj,\text{out}}$, takes the form

$$\gamma_{12}^{kj} = \sigma_{kj} \frac{M_{j}}{m_{j}} n_{c,k} n_{c,j} \hat{v}_r \int d\Omega \frac{4\pi}{\varepsilon_{j}} f_1^k f_1^j (f_1^j + 1),$$

(8)

with $\hat{v}_r$ the relative velocity and $M_{j}^{-1} = m_{j}^{-1} - m_{j}^{-1}$.

Figure 3 shows the equilibrium condensate and thermal density profiles (top panels) and collision rates (middle and bottom panels) for a mixture of $^{87}\text{Rb}$ (thin red lines) and $^{41}\text{K}$ (thick blue lines) at a temperature of $T = 21 \text{ nK}$, when condensate fractions $\approx 80\%$, for both miscible ($\Lambda = 0.3$, left column) and immiscible ($\Lambda = 2.3$, right column) cases. The two condensates (dashed lines) mix (top panel, left) or phase-separate (top panel, right) with thermal clouds (solid lines) displaying peaks at the condensate edges, thus also leading to a mean-field-induced double-peaked thermal structure. The spatially resolved collision rates between condensate and thermal atoms. Bottom: Spatially resolved collision rates between thermal atoms.
The significance of the $C^{ij}_{12}$ collisional terms may play during various sympathetic cooling stages.

The evaluation of integrated collision rates enables us to define a typical collisional time scale, $\tau = \int d\Gamma(r)/N_{\text{coll}}$, where $N_{\text{coll}}$ is the relevant number of available thermal atoms taking part in collisions for each process; this allows us to distinguish between the collisionless $[(\omega \tau)^{-1} < 1]$ and the hydrodynamic $[(\omega \tau)^{-1} > 1]$ regimes [31,42]. Figure 4(c) shows the variation of the hydrodynamic parameter $(\omega \tau)^{-1}$ for $^{87}$Rb-41K mixtures in the miscible (left) and immiscible (right) regimes, focusing only on interspecies collisions: this reveals the dominance of $(\omega \tau C)^{-1}$, which approaches 1 in the immiscible case, with all intraspecies collisions satisfying $10^{-2} < (\omega \tau C)^{-1} < 10^{-1}$ in both cases. Doubling the trap frequency to $2\pi \times 40$ Hz roughly doubles $(\omega \tau C)^{-1}$, increases $(\omega \tau C)^{-1}$ by $\approx 50\%$, and only slightly increases $(\omega \tau C)^{-1}$, which however remains the largest. Consideration of realistic $^{87}$Rb-$^{85}$Rb mixtures (characteristic values shown in Table I) reveals that while $(\omega \tau C)^{-1} \sim 1$ is always the largest interspecies contribution, tuning the intraspecies $\Delta_{\text{Rb85-Rb85}}$ to $900\hbar\omega$ [11] provides a plausible candidate for multicomponent hydrodynamic behavior in the sense of $(\omega \tau C)^{-1} \sim (\omega \tau C)^{-1} \sim 1$.

Conclusions. We have presented a system of coupled kinetic equations for the evolution of two-component condensates in the presence of dynamical thermal clouds. Analytical considerations led to the identification of a cross-condensate-exchange term, which was numerically shown to dominate, even at relatively high temperatures, over other collisional terms close to equilibrium, for both $^{87}$Rb-41K and $^{87}$Rb-$^{85}$Rb mixtures. Such a term could be highly relevant during sympathetic cooling, particularly in later stages, when the sympathetically cooled component acquires appreciable condensation. Consideration of collisional time scales indicated the potential of generating hydrodynamic multicomponent condensates with $(\omega \tau)^{-1} \sim 1$, at least for some collisional processes. Our work, which is generalizable to multicomponent Bose gases and Bose-Fermi mixtures, sets the scene for future dynamical studies of sympathetic cooling, multicomponent condensate formation, and coupled expansion dynamics.

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