Editors' Suggestion

Can Three-Body Recombination Purify a Quantum Gas?

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Three-body recombination in quantum gases is traditionally associated with heating, but it was recently found that it can also cool the gas. We show that in a partially condensed three-dimensional homogeneous Bose gas three-body loss could even purify the sample, that is, reduce the entropy per particle and increase the condensed fraction η. We predict that the evolution of η under continuous three-body loss can, depending on small changes in the initial conditions, exhibit two qualitatively different behaviors—if it is initially above a certain critical value, η increases further, whereas clouds with lower initial η evolve towards a thermal gas. These dynamical effects should be observable under realistic experimental conditions.

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In ultracold atomic gases, uncontrollable particle loss is usually associated with mundane and adverse effects, such as increase of temperature and entropy per particle. However, it can also have more interesting consequences [1]. In a 3D weakly interacting homogeneous Bose gas, one-body loss due to collisions with the background gas in the vacuum chamber results in the quantum analogue of Joule-Thomson cooling [3,4]. This is a purely quantum-statistical effect, with the only role of weak interactions being to ensure thermalization of the gas. Recently, it was also observed that in interaction-dominated 1D Bose gases atom loss led to cooling even though its origin was three-body recombination, which is traditionally associated with heating [5]. In these experiments [4,5], losses reduced the gas temperature, but they still made the samples *less degenerate*, because the fractional drop of the degeneracy temperature, set by the gas density, was even larger.

In this Letter, we show that in a partially condensed, weakly interacting homogeneous 3D Bose gas, three-body recombination can result in an intricate dynamical phase diagram; under certain conditions it can both cool and purify the gas, i.e., reduce the entropy per particle and increase the condensed fraction η. An ideal-gas thermodynamic calculation gives that the evolution of the system depends on whether η is above or below a critical value $\eta^* = 0.76$. For $\eta < \eta^*$, the gas cools but $\eta \to 0$. However, for $\eta > \eta^*$ the gas undergoes self-purification and $\eta \to 1$. This behavior is a consequence of the interplay of two quantum-statistical effects—saturation of the thermal cloud [4,6] and preferential loss of thermal atoms due to boson bunching [7–10] (see Fig. 1). Purification occurs not just despite the three-body nature of the loss, but specifically because of it. Considering the effects of weak two-body interactions on the thermodynamics, we find a more complex phase diagram, but qualitatively similar behavior for $na^3 < 10^{-7}$, where n is the gas density and a the s-wave scattering length.

These effects could be observed in a homogeneous Bose gas, produced in an optical box trap [11], near a zero crossing of a associated with a Feshbach resonance [12]. For both the saturation of the thermal component and the beneficial effects of boson bunching for purification, it is important that the gas is homogeneous, with the condensed and thermal components completely spatially overlapped [13].

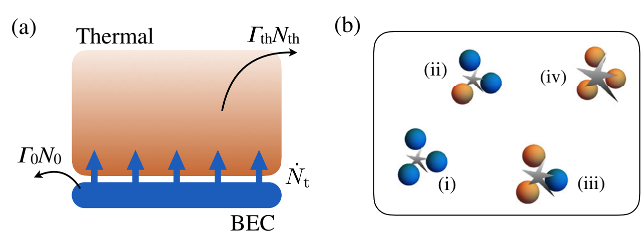

FIG. 1. Microscopic dynamics of an ideal homogeneous Bose gas with three-body loss. (a) Saturation-driven cooling. Loss of atoms from a saturated thermal cloud (at a rate $\Gamma_{th}N_{th}$) induces a flow of zero-energy atoms ($\dot{N}_t$) from the BEC to the thermal gas, which lowers the temperature. Direct loss of the BEC atoms ($\Gamma_0 N_0$) has no effect on the temperature. (b) Three-body loss processes. The rates of three-body collisions between different numbers of BEC (blue) and thermal (orange) atoms involve different combinatorial terms, reflecting the boson bunching that occurs in a thermal cloud but not in a BEC. Normalized by the appropriate powers of BEC and thermal densities, the relative rates of the processes (i)–(iv) are, respectively, $1/(3!)$, $1/(2!)$, 1, and 1. This preferential loss of thermal atoms can lead to purification of the gas.

The gas homogeneity also eliminates the problem of "anti-evaporation" heating present in harmonic traps [15], where the density dependent recombination preferentially removes atoms with below-average energy. We assume that three-body recombination is the dominant loss process and that loss products leave the box without undergoing secondary collisions. At the end of the Letter we discuss how these requirements can be fulfilled.

To elucidate the key physics, we start with an ideal-gas calculation, assuming that continuous thermalization is the only effect of two-body interactions.

In Fig. 1(a) we outline the idea of saturation-driven cooling. In a partially condensed ideal Bose gas of N atoms at temperature T, the thermal atom number $N_{\rm th}$ is saturated at the critical value for condensation $N_{\rm c}(T) \propto T^{\alpha}$, with $\alpha = 3/2$, and there are $N_0 = N - N_{\rm c}$ zero-energy atoms in the Bose-Einstein condensate (BEC). The total energy is $E \propto N_{\rm th} T \propto T^{\alpha+1}$ and the entropy per particle is proportional to the thermal fraction $1 - \eta = N_{\rm th}/N$ [6]. Removing BEC atoms through some loss process, at a rate we write as $\Gamma_0 N_0$, although Γ_0 may not be a constant, does not change E, $N_{\rm th}$, or T. However, removing thermal atoms through some (same or different) loss process, at a rate $\Gamma_{\rm th} N_{\rm th}$, reduces the energy according to $\dot{E}/E = -\Gamma_{\rm th}$. Since $T \propto E^{1/(\alpha+1)}$ and $N_{\rm th} \propto E^{\alpha/(\alpha+1)}$ depend only on E, we get

$$\frac{\dot{T}}{T} = -\frac{1}{\alpha+1}\Gamma_{\rm th} < 0 \quad \text{and} \quad \frac{\dot{N}_{\rm th}}{N_{\rm th}} = -\frac{\alpha}{\alpha+1}\Gamma_{\rm th}. \quad (1)$$

Note that $\dot{N}_{\rm th}/N_{\rm th} = -(3/5)\Gamma_{\rm th} \neq -\Gamma_{\rm th}$. To maintain equilibrium, with $N_{\rm th}$ saturated, atoms transfer between the BEC and the thermal cloud, at a rate $\dot{N}_t$, so the net rates of change of N_0 and $N_{\rm th}$ are $\dot{N}_0 = -\Gamma_0 N_0 - \dot{N}_t$ and $\dot{N}_{\rm th} = -\Gamma_{\rm th} N_{\rm th} + \dot{N}_t$. Specifically, for every 5 atoms lost from the thermal cloud, 2 are replenished from the BEC. This injection of zero-energy particles into the thermal cloud is the microscopic origin of the cooling.

These arguments are not specific to any particular loss process. They apply to the three-body loss discussed here and the one-body loss that drives the quantum Joule-Thomson effect observed in Ref. [4], and are also at the heart of the decoherence-driven cooling observed in Refs. [16,17], although in that case the atoms were not lost, but transferred to a different spin state.

To see whether atom loss can purify the gas, we calculate

$$\frac{\dot{\bar{\eta}}}{\bar{\eta}} = \frac{\dot{N}_{\rm th}}{N_{\rm th}} - \frac{\dot{N}}{N} = \Gamma(1 - \mathcal{P}), \quad (2)$$

where $\bar{\eta} = 1 - \eta$ is the thermal fraction, $\Gamma = -\dot{N}/N = (N_0\Gamma_0 + N_{\rm th}\Gamma_{\rm th})/N$ is the total per-particle loss rate, and we have introduced a dimensionless purification coefficient

$$\mathcal{P} \equiv \frac{\dot{N}_{\rm th}/N_{\rm th}}{\dot{N}/N}, \quad \text{so} \quad \mathcal{P} - 1 = \frac{d[\ln(1-\eta)]}{d[\ln(N)]}. \quad (3)$$

For $\mathcal{P} > 1$ the gas purifies ($\dot{\eta} > 0$), whereas for $0 < \mathcal{P} < 1$ it cools without purifying. From Eq. (1), for an ideal gas

$$\mathcal{P} = \frac{\alpha}{\alpha+1}\frac{\Gamma_{\rm th}}{\Gamma} = \frac{3}{5}\frac{\Gamma_{\rm th}}{\Gamma}, \quad (4)$$

so purification requires $\Gamma_{\rm th}/\Gamma > 5/3$. Here the nature of the loss process is crucial. One-body losses do not distinguish BEC and thermal atoms, so $\Gamma_{\rm th} = \Gamma_0 = \Gamma$ and $\mathcal{P} = 3/5$. However, for three-body loss $\mathcal{P}$ can be larger than 1.

In general, the local three-body loss rate is given by

$$\dot{n}/n = -g_3 K_3 n^2, \quad (5)$$

where g_3 is the zero-distance three-body correlation function and K_3 is the three-body loss coefficient. In terms of local condensate and thermal density, n_0 and $n_{\rm th}$, respectively [7],

$$g_3 = \frac{3!}{n^3}\left(\frac{1}{3!}n_0^3 + \frac{1}{2!}3n_0^2 n_{\rm th} + 3n_0 n_{\rm th}^2 + n_{\rm th}^3\right). \quad (6)$$

For a uniform gas, where $n_0/N_0 = n_{\rm th}/N_{\rm th} = n/N = 1/V$, with V being the gas volume, this corresponds to

$$\Gamma = K_3 n^2 (6 - 9\eta^2 + 4\eta^3). \quad (7)$$

For the same N and V, the loss rate in a pure BEC ($\eta = 1$) is 6 times smaller than in a thermal gas ($\eta = 0$), due to suppression of boson bunching [7,8]. More generally, the four terms on the right-hand side of Eq. (6) correspond, left to right, to the four loss processes (i)–(iv) in Fig. 1(b). Considering how many thermal and BEC atoms are lost in each process and keeping the same order of terms as in Eq. (6):

$$\Gamma_0 N_0 = K_3(N_0^3 + 6N_0^2 N_{\rm th} + 6N_0 N_{\rm th}^2 + 0)/V^2,$$
$$\Gamma_{\rm th} N_{\rm th} = K_3(0 + 3N_0^2 N_{\rm th} + 12 N_0 N_{\rm th}^2 + 6N_{\rm th}^3)/V^2,$$

corresponding to

$$\Gamma_0 = K_3 n^2 (6 - 6\eta + \eta^2),$$
$$\Gamma_{\rm th} = K_3 n^2 (6 - 3\eta^2). \quad (8)$$

Finally, inserting Γ and $\Gamma_{\rm th}$ into Eqs. (1), (2), (4), we obtain

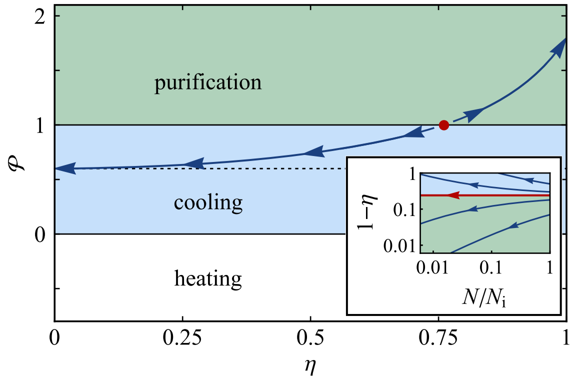

FIG. 2. Three-body cooling and purification of an ideal partially condensed homogeneous Bose gas. The purification coefficient $\mathcal{P}$ (see text), which determines whether the gas purifies ($\mathcal{P} > 1$) or cools without purifying ($0 < \mathcal{P} < 1$), depends only on the condensed fraction η. The critical value $\eta^* = 0.76$ (indicated by the red dot) defines a "bifurcation point" for the evolution of the cloud. As indicated by the arrows, for $\eta < \eta^*$ the condensed fraction keeps dropping, but for $\eta > \eta^*$ the gas self-purifies and $\eta \to 1$. The horizontal dashed line, $\mathcal{P} = 3/5$, corresponds to the result for one-body loss, which cannot purify the gas. Inset: evolution of η for different initial conditions; here N_i is the initial atom number.

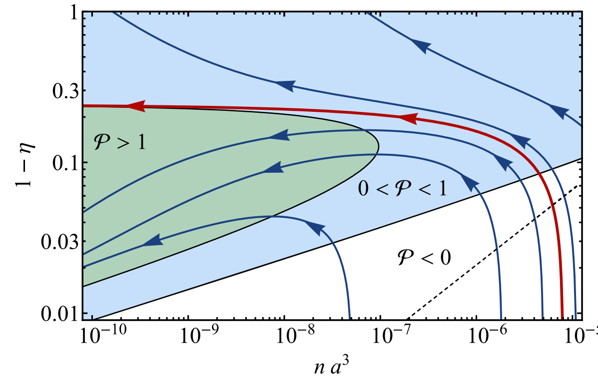

FIG. 3. Cooling and purification in a weakly interacting gas. The purification coefficient $\mathcal{P}$ now depends on the condensed fraction η and the gas parameter na^3. The evolution of the system is described by trajectories that flow either to $\eta = 1$ or to $\eta = 0$, depending on which side of the critical trajectory $\eta^*(na^3)$ (red line) they are. On this log-log graph the slope of the trajectories is given by $\mathcal{P} - 1$ [see Eq. (3)] and the background shading indicates whether instantaneously the gas purifies (green), cools without purifying (blue), or heats (white). In the regime below the dashed line, which corresponds to $k_B T = 2gn$, the dynamics could deviate from our results due to phononic nature of the thermal excitations.

$$
\begin{aligned}
\frac{\dot{T}}{T} &= -K_3 n^2 \frac{6}{5}(2-\eta^2), \\
\frac{\dot{\bar{\eta}}}{\bar{\eta}} &= -K_3 n^2 \frac{4}{5}(-3+9\eta^2-5\eta^3), \\
\mathcal{P} &= \frac{9}{5}\frac{2-\eta^2}{6-9\eta^2+4\eta^3}.
\end{aligned}
\tag{9}
$$

We see that $\mathcal{P}$ depends only on the condensed fraction η. As shown in Fig. 2, it monotonically grows from $3/5$ at $\eta = 0$ to $9/5$ at $\eta = 1$ [18]. For very small η, from $N \approx N_\mathrm{th}$ it directly follows that $\Gamma \approx \Gamma_\mathrm{th}$ and $\mathcal{P} \approx 3/5$. In this regime also $\Gamma_0 \approx \Gamma_\mathrm{th} \approx 6K_3 n_\mathrm{th}^2$. Microscopically, in this regime the two dominant processes in Fig. 1(b) are (iii) for the loss of BEC atoms and (iv) for the loss of thermal ones. These involve at most one BEC atom and hence have the same combinatorial factors, so $\Gamma_0 \approx \Gamma_\mathrm{th}$, and we essentially get the quantum Joule-Thomson effect [4], although driven by three-body loss. In the opposite limit $\eta \approx 1$, where $N \approx N_0$ and $\Gamma \approx \Gamma_0$, the two relevant processes in Fig. 1(b) are (i) and (ii), which have different combinatorial factors, such that $\Gamma_\mathrm{th} \approx 3\Gamma_0 \approx 3\Gamma$, giving $\mathcal{P} \approx 9/5$.

Crucially, $\mathcal{P} - 1$ changes sign at a critical condensed fraction $\eta^* = 0.76$; this is the only physical solution (satisfying $0 \le \eta \le 1$) to the cubic equation obtained by setting $\dot{\bar{\eta}} = 0$ in Eq. (9). As indicated by the arrows in Fig. 2, for $\eta < \eta^*$ the gas cools but $\eta \to 0$, while for $\eta > \eta^*$ the gas keeps self-purifying and $\eta \to 1$. This is illustrated in the inset of Fig. 2, where we show the evolution of the thermal fraction for different initial condensed fractions. On this log-log plot, $\mathcal{P} - 1$ gives the slope of the $\bar{\eta}(N)$ trajectories; see Eq. (3).

These ideal-gas effects should play a dominant role if the interaction energy is small compared to the thermal one. Within mean-field theory (see below), for small thermal fraction the ratio of thermal to interaction energy is $\approx 0.4\bar{\eta}^{5/3}/(na^3)^{1/3}$ [6], so the two are comparable for $\bar{\eta} = (na^3)^{1/5}$.

We now quantitatively assess the effects of weak two-body interactions on three-body cooling and purification, for $na^3 \lesssim 10^{-5}$ (see Fig. 3). In this regime, to a good approximation, interaction energy is mean-field like, g_3 is ideal-gas like [7,10], and the saturation picture holds [19]. We also assume that the thermal excitations are particlelike, which is a good approximation for most of the range of system parameters we consider (see dashed line in Fig. 3). The total energy is now

$$
E = \alpha_0 N_\mathrm{th} k_B T + \frac{g}{2V}(N_0^2 + 4N_0 N_\mathrm{th} + 2N_\mathrm{th}^2). \tag{10}
$$

Here $\alpha_0 = \alpha\zeta(\alpha+1)/\zeta(\alpha) = 0.77$, where ζ is the Riemann function, and $g = 4\pi\hbar^2 a/m$, where m is the atom mass.

A subtle question is how much interaction energy is removed from the gas through atom loss. Let us first consider an initially pure BEC, with $E = gN_0^2/(2V)$. For the BEC to stay pure after removal of a particle, the energy removed would have to be $\mu = \partial E/\partial N_0$. This would correspond to removing a particle adiabatically from a delocalized wave function. In contrast, a sudden local atom loss should simply remove the average energy per particle, $E/N_0 = \mu/2$. The gas is then left with total energy larger, by $\mu/2$, than that of a pure BEC with $N_0 - 1$ atoms, so this loss leads to heating. The next conceptual step is to extend this analysis to nonzero T. We rewrite Eq. (10) as

$$E = \left[\frac{g}{V}\left(\frac{1}{2}N_0 + N_{\mathrm{th}}\right)\right]N_0 + \left[\alpha_0 k_B T + \frac{g}{V}(N_0 + N_{\mathrm{th}})\right]N_{\mathrm{th}}$$

and interpret the terms in square brackets as the energy per BEC atom, ε_0 (left bracket), and the energy per thermal atom, $\varepsilon_{\mathrm{th}}$ (right bracket), in the sense that the rate of energy change should be

$$\dot{E} = -\varepsilon_0 \Gamma_0 N_0 - \varepsilon_{\mathrm{th}} \Gamma_{\mathrm{th}} N_{\mathrm{th}}. \quad (11)$$

Under continuous equilibration it must also be

$$\dot{E} = \frac{\partial E}{\partial N_0}(-\Gamma_0 N_0 - \dot{N}_t) + \frac{\partial E}{\partial N_{\mathrm{th}}}(-\Gamma_{\mathrm{th}} N_{\mathrm{th}} + \dot{N}_t), \quad (12)$$

where $\dot{N}_t$ is such that N_{th} remains saturated, and it can now in general be of either sign. Combining these equations gives the purification coefficient $\mathcal{P}$, a generalization of Eq. (9), which now depends on two dimensionless parameters, η and na^3:

$$\mathcal{P} = \frac{9(2-\eta^2) + b_1(\eta)(na^3)^{1/3}}{5(6 - 9\eta^2 + 4\eta^3) + b_2(\eta)(na^3)^{1/3}}, \quad (13)$$

where $b_1(\eta) = \gamma(7\eta^4 - 20\eta^3 + 12\eta^2 + 12\eta - 12)(1-\eta)^{-5/3}$ and $b_2(\eta) = 2\gamma\eta(6 - 9\eta^2 + 4\eta^3)(1-\eta)^{-2/3}$, with $\gamma = 2\zeta(3/2)^{5/3}/\zeta(5/2) = 7.4$.

In Fig. 3 we show examples of trajectories $\eta(na^3)$ for fixed (arbitrary) a. The red-colored trajectory separates those that flow to $\eta = 0$ and $\eta = 1$. The background shading indicates whether the gas instantaneously purifies ($\mathcal{P} > 1$), cools but does not purify ($0 < \mathcal{P} < 1$), or heats ($\mathcal{P} < 0$) [20].

At low thermal fraction $\bar{\eta}$, the constant-$\mathcal{P}$ contours in Fig. 3 follow the scaling $\bar{\eta} \propto (na^3)^{1/5}$, meaning that $\mathcal{P}$ is determined by the ratio of thermal and interaction energies. Qualitatively, affinity between particles (due to quantum statistics) leads to cooling, while aversion (due to repulsive interactions) leads to heating, similarly to how Joule-Thomson rarefaction leads to cooling of attractive classical gases and noninteracting bosons, and heating of repulsive classical gasses and noninteracting fermions [3,4]; here, each of the two opposing effects dominates in a different regime. The $\mathcal{P} = 0$ contour is $\bar{\eta} \approx (na^3)^{1/5}$ all the way to $na^3 = 10^{-5}$, while the purification effect is less robust in presence of two-body repulsion, but is still possible for $na^3 < 10^{-7}$. Also note that a system trajectory cannot leave the purification region $\mathcal{P} > 1$, but can enter it because losses reduce na^3. We have considered particlelike excitations, while phononic excitations will dominate the system's evolution for small $T/(gn) \sim (\bar{\eta}/\sqrt{na^3})^{2/3}$, below the dashed line in Fig. 3.

Our theory could be tested near a zero crossing of a, associated with a Feshbach resonance, where K_3 is nonzero and nearly a-independent. For illustration, we assume $K_3 \approx 10^{-29}\ \mathrm{cm}^6/\mathrm{s}$, as observed in, e.g., ^{7}Li [21] and ^{39}K [22], initial $n = 10^{14}\ \mathrm{cm}^{-3}$ and $\eta = 0.9$, and $a = 10a_0$, where a_0 is the Bohr radius. For these parameters, $na^3 = 1.5 \times 10^{-8}$, our calculation gives $\mathcal{P} > 1$ (see Fig. 3), and $\Gamma \approx 0.1\ \mathrm{s}^{-1}$ would be sufficiently large to dominate over the one-body loss rate, which is in many experiments $< 0.01\ \mathrm{s}^{-1}$. The healing length would be $\xi = 1/\sqrt{8\pi n_0 a} \approx 1\ \mu\mathrm{m}$, so in a box of size $L \gtrsim 10\ \mu\mathrm{m}$ the BEC would be essentially homogeneous and occupy the same volume as the thermal gas. The mean free path would be $\ell = 1/(8\pi n a^2) \approx 1$ mm, so secondary collisions of the loss products should be negligible. Finally, for continuous thermalization we want $\Gamma_2 > 3\dot{T}/T$ [23], where $\Gamma_2 \approx \bar{\eta}\sqrt{8k_B T/(\pi m)}\,8\pi n a^2$ (for small $\bar{\eta}$) is the per-particle rate of elastic two-body collisions, and $\dot{T}/T = \mathcal{P}\Gamma/\alpha \approx \Gamma$ from Eqs. (3), (13). This final requirement would be marginally satisfied in a ^{39}K gas, and very comfortably in a ^{7}Li one. We note that the initial n we assume is a few times larger than what was already achieved in box traps, but is not unrealistic.

In conclusion, we have shown that, under realistic experimental conditions, three-body recombination can both cool and purify a homogeneous Bose gas. We have calculated a dynamical phase diagram which shows that the behavior of the system can be qualitatively altered by small changes in the initial conditions. An interesting extension of this work would be to investigate the regimes of stronger interactions and/or very low thermal fractions, where the phonon nature of the excitations plays a role, thus connecting our study with the analysis performed in Refs. [5,24].

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