Damping and revivals of collective oscillations in a finite-temperature model of trapped Bose-Einstein condensation

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We utilize a two-gas model to simulate collective oscillations of a Bose-Einstein condensate at finite temperatures. The condensate is described using a generalized Gross-Pitaevskii equation, which is coupled to a thermal cloud modelled by a Monte Carlo algorithm. This allows us to include the collective dynamics of both the condensed and non-condensed components self-consistently. We simulate quadrupolar excitations, and measure the damping rate and frequency as a function of temperature. We also observe revivals in condensate oscillations at high temperatures, and in the thermal cloud at low temperature. Extensions of the model to include non-equilibrium effects and describe more complex phenomena are discussed.

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The first experimental observation of Bose-Einstein condensation (BEC) in magnetically trapped alkali atoms in 1995 [1,2] was a precursor to an explosion of interest in the properties of weakly-interacting Bose gases. Much of the subsequent theory [3] has focused on the dynamics of the condensate, including phenomena such as collective excitations and vortex motion. In the limit of zero temperature, one can represent the condensate by a macroscopic wavefunction analogous to a classical field. In this case the behavior can be described in terms of the Gross-Pitaevskii (GP) equation, which has the form of a nonlinear Schrödinger equation. Extension of the description to finite temperatures, where one must include fluctuations upon the condensate wavefunction, is a considerable challenge. However, the motivation is clear, as such a description would allow direct comparison with experiments where a non-condensed thermal cloud is present, as well as revealing new phenomena such as damping of collective modes [4–10] and the decay of metastable vortices [11].

Amongst the most compelling evidence for the validity of the GP equation at low temperatures is its quantitative agreement with experiment for low-energy collective modes. However, experimental investigations at higher temperatures have proved far more elusive, where experiments have demonstrated marked frequency shifts and damping of the condensate modes in the presence of a significant non-condensed component [11]. Theoretical studies have tended to concentrate on one of two regimes, depending upon the density and temperature of the system. At high densities, where collisions are sufficiently rapid to force the system into local equilibrium, the dynamics of the condensate and thermal cloud can be described by a set of coupled hydrodynamical equations [13–15]. Damping mechanisms in this case are of a dissipative type (i.e. viscosity and thermal relaxation). For very dilute systems or at low temperatures the mean free path of the elementary excitations become comparable to the size of the system and collisions play only a minor role. Damping in this collisionless regime is not related to thermalization processes but to coupling between excitations, and can be described within the framework of mean-field theories [16]. The collisionless regime may be appropriate for the JILA experiments [3], while the MIT experiments lie between the collisionless and hydrodynamical regimes [11].

Here we present a simple model of a finite-temperature BEC system, and use numerical simulations to find the temperature-dependent frequency and damping of a quadrupole mode. Essentially, we utilize a two-fluid approach, where the ground-state condensate and low-energy, highly-occupied ‘classical’ modes are described by a generalized GP equation, while the thermal cloud, which is composed of higher-energy excitations, is simulated using a Monte Carlo approach. One advantage of this model is that we do not need to invoke strong assumptions about particle collision times, so that we can study the intermediate region between the collisionless and hydrodynamical regimes. We also consistently include the collective dynamics of the thermal cloud, which are particularly significant at temperatures near to the Bose transition. This aspect is often absent from other treatments, for example frequency calculations from solving Hartree-Fock-Bogoliubov (HFB) equations [16,17]. Finally, the model can potentially be extended to simulate more complex situations, such as vortex decay and response to time-dependent probes.

The generalized GP equation for the condensate wavefunction, \( \Psi(r, t) \), is written in the Popov approximation (i.e. the ‘anomalous’ density, \( \bar{\eta} = 0 \)) as [13]

\[
i\hbar \frac{\partial}{\partial t} \Psi(r, t) = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(r, t) + g |\bar{n}(r, t) + n_c(r, t)|^2 - i \Lambda(r, t) \right) \Psi(r, t), \tag{1}
\]

where \( \bar{n}(r, t) \) is the non-condensate density, while \( n_c(r, t) = |\Psi(r, t)|^2 \) is the condensate density (where the wavefunction is normalized to the number of condensate atoms, \( N_c \)). The condensate is subject to an external...
trap potential, $V(r, t) = m(\omega_x^2 r^2 + \omega_z^2 z^2)/2$, as well as mean-field effects arising from the thermal cloud and the remainder of the condensate. These interactions are parameterized by the coupling constant, $g = 4\pi\hbar^2a/m$, where $m$ is the atomic mass and $a$ is the s-wave scattering length. In this paper we shall concentrate on $^{87}$Rb, where $a = 5.5 \text{ nm}$. The dissipative term, $\Lambda(r, t)$, represents collisions that transfer atoms between the condensed and non-condensed components. Here we shall assume local equilibrium between the two components, so that this term vanishes, $\Lambda = 0$. Generalization of this model to include this effect will be the subject of future work.

Given the non-condensate density $\hat{n}$ as a function of position and time, the GP equation (4) can be solved using techniques discussed in our previous work [18]. Briefly, the GP equation is re-scaled for convenience, before being propagated over a small time-step $\Delta t$ using a FFT method. The time-independent problem, corresponding to finding initial conditions of our simulations, can be solved by propagating in imaginary time, so that an arbitrary wavefunction quickly diffuses to the ground state solution. The equilibrium thermal distribution can be calculated under a semi-classical approximation [19], corresponding to the energy of a single particle moving within momentum states then simply yields

$$\hat{n}(r) = \frac{1}{\Lambda/T} g_3/2(z),$$

(2) where $z = \exp[-\beta \{V(r) + 2g(n_c(r) + \hat{n}(r)) - \mu\}]$ is the fugacity, $\Lambda/T = (2\pi\hbar^2/mk_BT)^{1/2}$ is the thermal wavelength, and $g_3(z) = \sum_{l=1}^{\infty} z^l / l^3$. The total number of atoms in the system is then given by $N = N_c + \int \text{d}r \hat{n} = N_c + \hat{N}$, where $\hat{N}$ is the number of atoms in the thermal cloud.

Self-consistent solution of (4) and (5) yields good approximations for the condensate and non-condensate densities at equilibrium. In particular, we iterate using successive evaluations of (5) and imaginary time propagation of the condensate wavefunction, to find the densities as a function of $N$ and $T$. Given this initial condition, the system dynamics resulting from a varying trap potential can be found by solving the time-dependent GP equation using propagation in real time. However, the problem of finding the non-condensate density becomes more challenging as this is also time-dependent. Under the semi-classical and Hartree-Fock approximations, and the assumption that the effective potential $U_{\text{eff}}(r, t) = V(r, t) + 2g(n_c(r, t) + \hat{n}(r, t))$ varies slowly in space, one can show (18) that the cloud of quasi-particle excitations may be described using a Boltzmann kinetic equation

$$\frac{\partial f(p, r, t)}{\partial t} + \frac{p}{m} \cdot \nabla f(p, r, t) - \nabla U_{\text{eff}} \cdot \nabla f(p, r, t) = \frac{\partial f}{\partial t}_{\text{coll}}.$$

(3)

The relationship between the phase-space distribution function $f(p, r, t)$ and the non-condensate density is simply given by

$$\hat{n}(r, t) = \int \frac{dp}{(2\pi\hbar)^3} f(p, r, t).$$

(4)

The right-hand term of (3), which provides the scattering rate of state $p$, is given by an integral representing two-body collisions between atoms in the thermal cloud within the Born approximation

$$\frac{\partial f}{\partial t}_{\text{coll}} = \frac{2g^2}{(2\pi\hbar)^3} \int dp_2 \int dp_3 \int dp_4 \delta(p_2 + p_4 - p_3) \delta(\epsilon_{p_2} + \epsilon_{p_3} - \epsilon_{p_1}) \times [(1 + f_1)(1 + f_2)f_3f_4 - f_1(1 + f_3)(1 + f_4)],$$

(5)

with $f = f(p, r, t)$ and $f_i = f(p_i, r, t)$. Locally, an excited atom has the HF energy $\epsilon_{p_2}(r, t) = p_2^2/2m + U_{\text{eff}}(r, t)$. As above, we neglect collisions that transfer atoms between the two components. The collision integral (5) differs from that of a classical gas [20] by the inclusion of $(1 + f)$ factors that represent Bose enhancement of scattering into occupied states.

In Refs. [3–5], moments of the kinetic equation (5) were taken to yield hydrodynamical equations [21]. These can be solved explicitly under certain conditions using a variational method [21]. An alternative approach is to solve (5) directly. In general, this is very difficult owing to the six-dimensional nature of phase space. One possibility is to work under the assumption of sufficient ergodicity. Ergodicity assumes that the distribution of atoms in phase space depends only on their energy, $\hat{e}$. Then (5) reduces to an equation of motion for $f(\hat{e})$. This assumption is well-known in the literature and has been used to model evaporative cooling [22, 23] and condensate growth [24–26] in Bose gases. However, ergodicity assumes that any deformation in momentum or position space is isotropic, or that the ergodic mixing time is shorter than the elastic collision time. In general non-ergodic situations this assumption is not valid. In addition, we are primarily interested in the gas dynamics in position space and its coupling to the condensate. Hence, a Monte Carlo technique [27–29] is more appropriate here. In particular, we utilize a direct simulation Monte Carlo (DSMC) method, as performed to model evaporative cooling in Bose gases [28, 29], and described in detail for classical gas dynamics in [30]. We now discuss our extension of this model to simulate the thermal cloud coupled to the condensate.

The direct simulation Monte Carlo (DSMC) method was first developed by Bird to describe classical gas flows [30]. It is equivalent to solving the Boltzmann equation
in phase-space, except that it recognizes the discrete nature of the gas on a microscopic level. In principle, the trajectory of each atom could be followed at all times, so that the state of the system is completely described by storing \((r,v)\) for all atoms. However, the calculation becomes unfeasible in the presence of interparticle collisions. Bird’s method makes the key assumption that the free particle motion and collisions are uncoupled over a short time interval, \(\Delta t\). This provides an accurate description of the gas so long that \(\Delta t < \tau_{\text{coll}}\), where \(\tau_{\text{coll}}\) is the mean collision time. Hence the DSMC method is most appropriate for describing gases in the Knudsen regime, where the mean free path is much larger than the size of the system. The technique is therefore well suited to dilute alkali gases.

First, the atoms are moved over distances appropriate to their velocity components, \(v_k\) \((k \in \{x, y, z\})\), such that \(r_{k+1} = r_k + v_k \Delta t\), before collisions are treated. To ensure that collisions only take place between near neighbours, position space is divided into cubic cells of a size much smaller than the dimensions of the cloud. The number of atoms is counted in each cell to furnish the local density \(\bar{n}(r)\). Pairs of atoms in a cell are then chosen at random, and the momenta after a collision is calculated \(a \text{ priori}\). To account for energy and momentum conservation the collision is most conveniently treated in the atomic centre-of-mass frame. Two further random numbers, \(R_1\) and \(R_2\), are chosen to determine the scattering angles \(\phi = 2\pi R_1\) and \(\theta = 1 - 2R_2\), where \(R_{1,2} \in [0, 1]\).

To decide whether the atoms actually do collide, the following algorithm is used. First, the mean number of collisions locally in time \(\Delta t\) is calculated using

\[
\dot{\rho}(r,t) = \bar{n}(r,t) \sigma v_e \Delta t \left[ 1 + f(p_3, r, t) \right] \left[ 1 + f(p_4, r, t) \right],
\]

where \(\sigma = 8 \pi a^2\) is the scattering cross-section for bosons in a hard sphere model, and \(v_e = |v_2 - v_1|\) is the relative velocity of the two atoms. A ‘quantum scattering factor’ is also included which represents the effect of Bose statistics, where \(p_3\) and \(p_4\) are the momenta of the collision products. To estimate the distribution function, the number of atoms are counted within subcells in momentum space, which in turn are subdivisions of the positional cells. Strictly speaking, each phase-space subcell should have a volume of \(\hbar^3\), which is the minimum value allowed by the uncertainty principle. However, the computational time required to sort the atoms increases linearly with the total number of subcells, and can become prohibitively large without some form of coarse graining. We therefore count the number of atoms \(N_{\text{sc}}\) within larger subcells, which is renormalized to yield \(f(p, r, t) \approx N_{\text{sc}} \hbar^3 / V_{\text{sc}} v_i\), where \(V_i\) and \(V_{\text{sc}}\) are the volumes of cells in momentum and position space respectively. We find that our results are largely independent of the number of cells and subcells for sufficiently large numbers. For example, for the computations described below we use 8000 position cells subdivided into 9261 momentum subcells.

As \(\rho(r,t) \ll 1\), the collision probability is given by \(P_{\text{coll}} = 1 - e^{-\dot{\rho}(r,t)}\). A further random number, \(R_{\text{c}} \in [0, 1]\), is compared to \(P_{\text{coll}}\). Only if \(R_{\text{c}} < P_{\text{coll}}\) does a collision takes place. Once this procedure has been repeated for all of the atoms in each cell, the final part of the time-step involves updating the atom velocities to account for gradients in the external potential, \(v_{k+1} = v_k + \Delta v_k\), where \(\Delta v_k = -\partial_k U_{\text{eff}} \Delta t / m\).

To simulate the coupled system, alternating Monte Carlo and GP propagation steps are performed during each time-step, \(\Delta t\), where thermal atoms move in the mean-field potential, \(U_{\text{eff}}\). The thermal gas density is calculated at all points by counting atoms in each cell. The cells do not necessarily correspond to the GP grid, so cubic spline interpolation is used to smooth \(\bar{n}\). This prevents discontinuities in the mean-field potential, that may lead to instabilities in the FFT method used to propagate the condensate wavefunction.

The first stage of the simulation is to find the initial state for a prescribed temperature, \(T\). The numbers of condensate and thermal atoms are found by the semi-classical algorithm described above. The equilibrium condensate density evaluated by this method, as well as a Maxwell-Boltzmann distribution for the thermal atoms, are used as an initial state for the MC-GP algorithm. The condensate is propagated through imaginary time while the thermal cloud relaxes to equilibrium. A time-dependent trap potential \(V(r,t)\) is applied and the system allowed to propagate in real time.

We simulate collective excitations of \(N = 40000\) atoms in a disk-shaped trap (\(\omega_r = 2\pi \times 131\) Hz, \(\omega_z = \sqrt{8\omega_r}\)). These are similar parameters to the JILA experiment [4]. We study the \(m = 0\) quadrupole mode, which is excited by a sudden 10% increase in the radial frequency, \(\omega_r [31]\). The subsequent condensate oscillations are shown in Fig. 1. We clearly observe damping at higher temperatures, which is absent at \(T = 20\) nK. Note that we determine the widths of both the components by calculating the standard deviation \(\sigma_k = \sqrt{\langle k^2 \rangle - \langle k \rangle^2}\), where we use \(\langle k^2 \rangle = \int d^3r k^2 |\Psi|^2\) for the condensate and \(\langle k^2 \rangle = \sum k_i^2 / N\) for the thermal cloud. To avoid large statistical fluctuations in the thermal component, especially at low temperatures, we simulate ten times the physical number of atoms (equivalent to repeatedly running our simulations: a time-consuming process). For consistency the density and phase-space density of the gas are rescaled appropriately.

We fit the condensate widths along \(x\) and \(y\) to an exponentially decaying function: \(\sigma_k(t) = A e^{-\Gamma t} \cos \omega t + B\). The oscillation decay rate, \(\Gamma\), and frequency, \(\omega\), are plotted against temperature in Fig. 2. The damping increases from zero at low temperatures, before tending towards a linear dependence at intermediate values (\(T < 0.7T_c\)). This is in agreement with the expected behaviour of Landau damping in homogeneous and trapped condensates, where in the limit of zero temperature the damping has a \(\Gamma \sim T^4\) dependence, while at higher temperatures \(\Gamma \sim T^1\) [31, 32]. We also observe quantita-
tive agreement with previous theory and experiment in this regime. For example, at $T = 200 \text{nK}$ ($T/T_0 \simeq 0.7$) we find that $\Gamma \simeq 45.3 \text{s}^{-1}$, in fair agreement with the experimental value of $90 \pm 40 \text{s}^{-1}$ [6]. Landau damping arises due to mean-field coupling between fluctuations in the condensate wavefunction, $\delta \Psi$, and in the non-condensate density, $\delta n$. Physically this is equivalent to absorption of a quantum of the collective mode by a thermal excitation [13]. We find no damping at low temperatures, so that Balilev damping, which is active even at zero temperature, is not observed. This is to be expected, as the mechanism involves the decay of the collective mode into two lower frequency excitations and is equivalent to coupling between $\delta \Psi$ and fluctuations in the anomalous density, $\delta n$, which are neglected in our model. Nevertheless, the model is still consistent because Balilev damping is expected to be suppressed for the lowest modes in trapped condensates due to the discrete nature of the levels at low energy.

As shown in Fig. 3, the condensed and normal components oscillate at slightly different frequencies due to their weak coupling, and the condensate is much more highly damped than the thermal gas. The latter is a consequence of the more massive thermal cloud at this temperature (so that the back-action from Landau damping has less of an impact) and the small ‘internal’ damping of the cloud from thermalization processes. As a result the thermal cloud acts as a kind of energy reservoir. When the oscillations of the two components are in anti-phase the condensate oscillations are strongly damped; however, when they are in phase the thermal cloud tends to drive the condensate oscillations. This beating effect is most noticeable when one component is significantly larger than the other. Correspondingly, we see the same effect in the thermal cloud at low temperatures.

The condensate oscillation frequencies are also plotted in Fig. 2. The figure shows a small downward shift in frequency for $T < 0.67T_0$ [9,10,17,33]. An increase in frequency above $0.67T_0$ is also observed; however, this is not as large as that seen in the JILA experiment [9], where the frequency approaches $2\omega_x$ in this region. A possible explanation for the experimental behaviour was provided by Bijlsma and Stoof [35], who suggested a cross-over between normal modes where the two components oscillate in phase and anti-phase. However, as noted previously we find that the components oscillate at slightly different frequencies, and this description is inappropriate here. We may be able to see this effect at higher temperatures, though unfortunately the condensate in this regime is small and more sensitive to local fluctuations in the thermal cloud density, leading to unacceptable errors. The experimental data also suffers from large errors in this region, making a direct comparison difficult.

Note that the Landau damping observed here should not be confused with the damping mechanism discussed in [3,8], which is due to collisions that excite condensate atoms into the thermal cloud. For example, Landau damping is a three excitation process as opposed to the four excitations involved in collisional damping. Our approach is justified as a first approximation because for relevant parameters the magnitude of collisional damping is significantly smaller than Landau damping [31].

We observe a dip in the damping rate in the region $0.7T_0 < T < 0.87T_0$. This is related to an interesting ‘beating’ effect in the condensate oscillation. In this temperature range the oscillations are seen to damp rapidly at early times, before reviving at a smaller amplitude after approximately ten oscillations. As a result, the fitting function tends to underestimate the damping rate.
To summarize, we have studied frequency shifts and Landau damping due to mean-field coupling between the condensate and the thermal cloud. We also observe revivals in the condensate oscillations at high temperatures due to back-coupling from the thermal cloud, illustrating that damping is not completely irreversible. Future extensions to our Monte Carlo simulations could include collisions that excite atoms out of the condensate [14,15,34]. Along with a description of additional damping processes in collective excitations, this extended model could also be used to study condensate formation in systems far from equilibrium. Another application might consider vortex dynamics at finite temperatures. A vortex in this case would be an ‘obstacle’ in the mean-field experienced by non-condensed particles, leading to scattering and hence to a net force on the vortex. This should result in the expected drift of the vortex to the condensate edge, and allow direct determinations of vortex lifetimes. Similar models could also facilitate a fully consistent description of dissipative processes during probing of the condensate by a moving object [18].

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