We derive two different sets of rate equations for sympathetic cooling of harmonically trapped Bosons or Fermions. The rate equations are obtained from a master equation derived earlier by Lewenstein et al. [Phys. Rev. A 51 (1995) 4617] by means of decoherence and ergodicity arguments. We show analytically that the thermal equilibrium state is a stationary solution of our rate equation. We present analytical results for the rate coefficients which are needed to solve the rate equations, and we give approximate formulae that permit their computation in practice. We solve the two sets of rate equations numerically and compare the results. The cooling times obtained in both approaches agree very well. The equilibration rates show fair agreement.

**I. INTRODUCTION**

The cooling of atoms in traps is an important tool in the study of the behavior of systems of Bosons and Fermions at low temperatures. Usually, the last step in the cooling process is evaporative cooling. For this step to be efficient, thermodynamic equilibrium of the cooled gas must be (nearly) attained at all times. This condition is met if the atoms interact sufficiently strongly. There is a number of gases in which the interaction is too weak for evaporative cooling to work. In such cases, one resorts to “sympathetic cooling”: Another gas is cooled evaporatively. This gas acts as the cooling agent for the gas which is to be
cooled. It is usually legitimate to assume that the number of atoms in the cooling agent is very large, or that another mechanism is operative which keeps the cooling agent at fixed temperature. In either case, the cooling agent acts as a heat bath of fixed temperature.

The method of sympathetic cooling was proposed almost twenty years ago [1,2] and has since found widespread application (see Refs. [3,4]). Exciting recent applications include the sympathetic cooling of $^6$Li Fermions in a bath of $^7$Li Bosons [5,6], and the production of dual Bose–Einstein condensates with sympathetic cooling [7,8]. However, to the best of our knowledge, there does not exist until now a practicable theoretical description of this process. This gap is remarkable because theory would be expected to make predictions on the dependence of the cooling rate on various parameters defining both the interaction between atoms in the cooling agent and in the cooled gas, and on the trap potential, and might thus be helpful in improving the cooling process. We are aware of only two papers which deal with sympathetic cooling theoretically. Lewenstein et al. [9] derived a master equation for sympathetic cooling. Unfortunately, that master equation is too complex to be useful, see below. Geist et al. [10] have formulated sympathetic cooling of Fermi gases in terms of a quantum Boltzmann equation. The tremendous simplification of the collision matrix elements achieved in this way results, however, mainly in a qualitative description of the cooling process.

It is the purpose of the present work to derive rate equations for the cooling process which can be implemented and used practically. We do so by simplifying the master equation of Ref. [9] and by reducing it to a set of rate equations. We demonstrate the utility of our approach by presenting analytical and numerical results which apply to the cooling process. In the present Section, we begin by listing the assumptions and collecting the results of Ref. [9]. We use the notation of Ref. [9].

The cooling gas (referred to as system $B$) consists of Bosons in thermal equilibrium at temperature $T_B$. We use $\beta_B = (\kappa T_B)^{-1}$ where $\kappa$ is Boltzmann’s constant. It is assumed that $T$ does not change during the cooling process. It is also assumed that the atoms in system $B$ are much heavier than those of the cooled gas. The single–particle states of
system $B$ are then approximated by plane waves with energies $\varepsilon(k) = (\hbar \vec{k})^2/(2M)$ with $\vec{k}$ the momentum and $k = |\vec{k}|$, with corresponding creation and annihilation operators $b^\dagger(\vec{k})$ and $b(\vec{k})$, respectively. Summations over $\vec{k}$ are always replaced by integrations. The number $n(k)$ of particles with wave number $\vec{k}$ is given by

$$n(k) = \frac{z \exp[-\beta_B \varepsilon(k)]}{1 - z \exp[-\beta_B \varepsilon(k)]}$$

(1)

where $z$ denotes the fugacity. While we retain Eq. (1) in our analytical work, in the numerical work of Section [VII] below $T_B$ is taken to be so large that the coefficients $n(k)$ can be replaced by a Boltzmann distribution,

$$n(k) = n_B \Lambda_B^3 \exp[-\beta_B \varepsilon(k)]$$

(2)

with

$$n_B = (2\pi)^{-3} \int \mathrm{d}^3 k \ n(k)$$

(3)

the density of atoms in $B$ and $\Lambda_B = (2\pi \hbar^2 \beta_B / M)^{1/2}$ the thermal de–Broglie wave length of the atoms in system $B$. Again, Eq. (2) applies if the mass of the atoms in system $B$ is sufficiently large.

The atoms subject to sympathetic cooling (referred to as system $A$) are confined by a harmonic–oscillator potential with trap frequency $\nu$. We simplify the notation by confining ourselves to isotropic traps in three dimensions. The generalization to other dimensions, and to non–isotropic traps, is straightforward. The single–particle states in the harmonic–oscillator potential have quantum numbers $\vec{n} = n_x, n_y, n_z$. The integers $n_x, n_y, n_z$ are positive or zero and count the number of harmonic–oscillator quanta in the $x, y$ and $z$ directions of a Cartesian coordinate system. The single–particle eigenfunctions are labelled $\psi_{\vec{n}}(\vec{x})$, the eigenvalues $\epsilon_{\vec{n}}$. The corresponding creation and annihilation operators are denoted by $a_{\vec{n}}^\dagger$ and $a_{\vec{n}}$, respectively. Unless stated otherwise, we consider the atoms in system $A$ to be Bosons.

The interaction $H_{A-B}$ between atoms in system $A$ and those in system $B$ is described by the Hamiltonian
\[
H_{A-B} = \sum_{\vec{n},\vec{n}'} \int d\vec{k}d\vec{k}' \gamma_{\vec{n},\vec{n}'}(\vec{k}, \vec{k}') a_{\vec{n}}^\dagger a_{\vec{n}'} b(\vec{k}) b(\vec{k}') .
\]  

(4)

The matrix elements of the interaction are denoted by \( \gamma_{\vec{n},\vec{n}'}(\vec{k}, \vec{k}') \). These matrix elements contain the two-body interaction which is approximated by a delta function of strength

\[
C = \frac{4\pi \hbar^2 a}{2\mu}
\]

(5)

where \( a \) is the scattering length and \( \mu \) the reduced mass. Then, the matrix elements \( \gamma_{\vec{n},\vec{n}'}(\vec{k}, \vec{k}') \) are given by

\[
\gamma_{\vec{n},\vec{n}'}(\vec{k}, \vec{k}') = \frac{C}{(2\pi)^3} \int d^3 x \psi_{\vec{n}}(\vec{x}) \psi_{\vec{n}'}(\vec{x}) \exp \left[-i(\vec{k} - \vec{k}') \cdot \vec{x}\right].
\]

(6)

The rate coefficients \( \Gamma_{\vec{m},\vec{m}'}_{\vec{n},\vec{n}'} \) appearing in the master equation below are given by

\[
\Gamma_{\vec{m},\vec{m}'}_{\vec{n},\vec{n}'} = \frac{1}{2\hbar^2} \int_{-\infty}^{\infty} d\tau \int d^3 k d^3 k' \gamma_{\vec{n},\vec{n}'}(\vec{k}, \vec{k}') \gamma_{\vec{n}',\vec{n}'}(\vec{k}', \vec{k})
\]

\[
\times n(k) [n(k') + 1] \exp \left[ i(\varepsilon(k) - \varepsilon(k') + \alpha\hbar\nu) \tau / \hbar \right].
\]

(7)

The integer \( \alpha \) is defined by

\[
\alpha = (m'_x + m'_y + m'_z) - (m_x + m_y + m_z) = (n_x + n_y + n_z) - (n'_x + n'_y + n'_z).
\]

(8)

Obviously, \( \alpha \) can be positive, negative, or zero. The last relation in Eq. (8) restricts the possible values of \( \vec{m}, \vec{m}', \vec{n}, \vec{n}' \).

The master equation describes the dependence on time \( t \) of the reduced density matrix \( \rho_A(t) \) for system \( A \), obtained by tracing the total density matrix for systems \( A \) plus \( B \) over system \( B \). Under the assumptions that the process is Markovian and that the correlation time for the interaction between systems \( A \) and \( B \) is much shorter than the cooling time, and with the help of a rotating–wave approximation, the master equation takes the form

\[
\frac{d\rho_A(t)}{dt} = -\frac{i}{\hbar} \left[ H_A + H'_{A-A}, \rho(t) \right] + \mathcal{L} \rho_A .
\]

(9)

Here, \( H_A \) is the sum of the single–particle Hamiltonians for atoms in system \( A \) containing the kinetic energy and the harmonic–oscillator potential of the trap, while \( H'_{A-A} \) contains
the interaction between the atoms in system $A$. The action of the Liouvillean $\mathcal{L}$ on the reduced density matrix $\rho_A(t)$ is given by

$$\mathcal{L}\rho_A = \sum_{\vec{n},\vec{n}',\vec{m},\vec{m}'} \Gamma_{\vec{n},\vec{n}'}^{\vec{m},\vec{m}'} \left( 2a^\dagger_{\vec{n}} a_{\vec{n}} \rho_A(t) a^\dagger_{\vec{m}} a_{\vec{m}} - a^\dagger_{\vec{n}} a_{\vec{n}} a^\dagger_{\vec{m}} a_{\vec{m}} \rho_A(t) - \rho_A(t) a^\dagger_{\vec{n}} a_{\vec{n}} a^\dagger_{\vec{m}} a_{\vec{m}} \right). \quad (10)$$

Eqs. (9,10) are not useful as they stand. Even if the accessible single–particle states of the harmonic oscillator are restricted to the lowest 30 $\hbar \nu$ or so, the dimension of the resulting matrix representation of $\rho_A$ is enormous. Moreover, the numerical calculation of each of the rate coefficients $\Gamma_{\vec{n},\vec{n}'}^{\vec{m},\vec{m}'}$ presents formidable difficulties. These are compounded by the sheer number of such coefficients needed in the calculation. Thus, it is necessary to simplify Eqs. (9,10). We do so in a sequence of steps. In Section II, we show that the decoherence time $\tau_{\text{dec}}$ for the system $A$ is inversely proportional to $\sqrt{n_B}$ where $n_B$ is proportional to the number of particles in system $B$, see Eq. (3). Therefore, $\tau_{\text{dec}}$ is the smallest time scale in the problem. As a consequence, the off–diagonal elements of $\rho_A$ are damped out very quickly, and $\rho_A$ becomes diagonal in energy representation. The ensuing reduction of the number of equations and of rate coefficients is not yet sufficient, however, to lead to a practicable problem. We aim at a sufficiently simple rate equation. In Ref. [9] it was pointed out that the degeneracy of the harmonic–oscillator states causes difficulties in the conversion of the master equation into a rate equation. We overcome this problem by assuming that the interaction between atoms in system $A$, although weak, lifts this degeneracy. We investigate two independent possibilities of reducing the problem further. In Section III, we average the density matrix over all many–body states having, for $H'_{A-A} = 0$, the same excitation energy (a fixed multiple of $\hbar \nu$). The resulting rate equation connects diagonal matrix elements of $\rho_A$ in energy representation. Alternatively, we introduce a factorization assumption for the density matrix $\rho_A$ (Section IV). This procedure yields a simple and intuitively convincing form of the rate equation. The factorization assumptions used in Section IV and, more implicitly, also in Section III are kin to a mean–field approximation. In Section IV we check their validity by calculating the influence of the fluctuations on the rate equation which are
neglected in the mean-field approach. In Section [V], we test the consistency of our scheme. We show that the equilibrium distribution of Bosons in the ground state of system \( A \) derived from our rate equation coincides with the one calculated by Scully [I] from a different starting point. We then use our results for a numerical calculation. The rate coefficients are worked out in Section [VI]. The rate equations are solved, and the results are discussed in Section [VII]. Particular attention is paid to a comparison between results obtained in the framework of Section [III] and of Section [IV]. Section [VIII] contains the conclusions.

II. DECOHERENCE

The interaction with the heat bath (i.e., with system \( B \)) not only cools system \( A \) but also induces decoherence: The off-diagonal elements (in energy representation) of the reduced density matrix \( \rho_A(t) \) decay in time. In this Section, we estimate the decoherence time \( \tau_{\text{dec}} \) and show that \( \tau_{\text{dec}} \) is proportional to \( 1/\sqrt{n_B} \) and, thus, much shorter than all other time scales in the problem.

The common procedure [12] consists in calculating the time dependence of the linear entropy \( \delta_A(t) \) defined by

\[
\delta_A(t) = 1 - \text{tr}_A([\rho_A(t)]^2)
\]

in terms of a power-series expansion in \( t \), assuming that at time \( t = 0 \) the total density matrix \( \rho(0) \) of systems \( A + B \) obeys \( \rho(0) = \rho_A(0) \otimes \rho_B(0) \) with \( \text{tr}_A\rho_A(0) = \text{tr}_A(\rho_A(0))^2 = 1 \) and \( \text{tr}_B\rho_B(0) = 1 \). The decoherence time \( \tau_{\text{dec}} \) is given by the inverse of the coefficient multiplying \( t \) or, should this term vanish, by the square root of the inverse of the coefficient multiplying \( t^2 \). We face the second alternative because in Ref. [9] it is assumed that \( \text{tr}_B(\rho_B H_{A-B}) = 0 \).

This causes the term linear in \( t \) to vanish.

Second-order perturbation theory with respect to \( H_{A-B} \) yields

\[
\delta_A(t) = \frac{2}{\hbar^2} \int_0^t \text{d}t' \int_0^{t'} \text{d}t'' \text{tr}_A \left( \rho_A(0) \text{tr}_B \left( [\tilde{H}_{A-B}(t'), \left[ \tilde{H}_{A-B}(t''), \rho_A(0) \otimes \rho_B(0) \right] \right) \right). \tag{12}
\]
The tilde indicates that the operator is taken in the interaction representation. We focus attention on the trace over \( B \) and consider

\[
X = \text{tr}_B \left( \left[ \tilde{H}_{A-B}(t'), \tilde{H}_A(t'') \right], \rho_A(0) \otimes \rho_B(0) \right). \tag{13}
\]

With \( H_0 = H_A + H_B \) the sum of the Hamiltonians for the atoms in systems \( A \) and \( B \), \( X \) is explicitly given by

\[
X = \sum_{\vec{n}_1 \vec{n}_1'} \sum_{\vec{n}_2 \vec{n}_2'} \int d^3k_1 \int d^3k_1' \int d^3k_2 \int d^3k_2' \gamma_{\vec{n}, \vec{n}'}(k_1, k_1') \gamma_{\vec{n}_2 \vec{n}_2'}(k_2, k_2') Y \tag{14}
\]

where

\[
Y = \text{tr}_B \left( \left[ \exp(iH_0 t'/\hbar) a_{\vec{n}_1}^+ a_{\vec{n}_1'} b_{k_1}^+ b_{k_1'} \exp(-iH_0 t'/\hbar), \right. \right. \\
\left. \left. \left[ \exp(iH_0 t''/\hbar) a_{\vec{n}_2}^+ a_{\vec{n}_2'} b_{k_2}^+ b_{k_2'} \exp(-iH_0 t''/\hbar), \rho_A(0) \otimes \rho_B(0) \right] \right) . \tag{15}
\]

We define

\[
A_{\vec{n}_1 \vec{n}_1'}(t) = \exp(iH_A t/\hbar) a_{\vec{n}_1}^+ a_{\vec{n}_1'} \exp(-iH_A t/\hbar) \tag{16}
\]

and correspondingly for \( B_{\vec{k}_1 \vec{k}_1'}(t) \). A straightforward calculation yields

\[
Y = \left[ A_{\vec{n}_1 \vec{n}_1'}(t'), A_{\vec{n}_2 \vec{n}_2'}(t'') \rho_A(0) \right] \text{tr}_B \left( B_{\vec{k}_1 \vec{k}_1'}(t') B_{\vec{k}_2 \vec{k}_2'}(t'') \rho_B(0) \right) \]

\[
- \left[ A_{\vec{n}_1 \vec{n}_1'}(t'), \rho_A(0) A_{\vec{n}_2 \vec{n}_2'}(t'') \right] \text{tr}_B \left( B_{\vec{k}_1 \vec{k}_1'}(t') \rho_B(0) B_{\vec{k}_2 \vec{k}_2'}(t'') \right) . \tag{17}
\]

The two traces over \( B \) yield

\[
\text{tr}_B( B_{\vec{k}_1 \vec{k}_1'}(t') B_{\vec{k}_2 \vec{k}_2'}(t'') \rho_B(0)) = n(k_1)[n(k_2) + 1] \times \exp \left( i \left( \varepsilon(k_1) - \varepsilon(k_2) \right)(t' - t'') / \hbar \right) ,
\]

\[
\text{tr}_B( B_{\vec{k}_1 \vec{k}_1'}(t') \rho_B(0) B_{\vec{k}_2 \vec{k}_2'}(t'')) = n(k_2)[n(k_1) + 1] \times \exp \left( i \left( \varepsilon(k_1) - \varepsilon(k_2) \right)(t' - t'') / \hbar \right) . \tag{18}
\]

Inserting this result back into Eq. (17) and the latter into Eq. (14), performing the trace over \( A \), carrying out the time integrations, and expanding in powers of \( t \), we obtain to lowest non–vanishing order
\[ \delta_A(t) = \left( \frac{t}{\tau_{\text{dec}}} \right)^2 \]  

where 

\[
\left( \frac{1}{\tau_{\text{dec}}} \right)^2 = \frac{1}{\hbar^2} \sum \int d^3k_1 \int d^3k_2 |\gamma_{\vec{n}_1\vec{n}_2}(\vec{k}_1,\vec{k}_2)|^2 \times \left( n(k_1)[n(k_2) + 1]n(\vec{n}_1)[n(\vec{n}_2) + 1] \
+ n(k_2)[n(k_1) + 1]n(\vec{n}_2)[n(\vec{n}_1) + 1] \right).
\]

Here, \( n(\vec{n}) = \text{tr}_A(a^\dagger_{\vec{n}}a\rho_A(0)) \).

The terms containing the occupation numbers \( n(k) \) in Eq. (20) have the form 

\[ n(k_1)[n(k_2) + 1] = n(k_1)n(k_2) + n(k_1) \quad \text{and} \quad n(k_2)[n(k_1) + 1] = n(k_1)n(k_2) + n(k_2). \]

We focus attention on the terms linear in the occupation numbers and observe that the \( k \)-dependence of the remaining part of the integrand resides in \( |\gamma_{\vec{n}_1\vec{n}_2}(\vec{k}_1,\vec{k}_2)|^2 \). This quantity depends only on \( \vec{k}_1 - \vec{k}_2 \), see Eq. (4). In the term linear in \( n(k_1) \) \( (n(k_2)) \), we introduce the integration variables \( \vec{k}_1 \) and \( \vec{\kappa} = \vec{k}_1 - \vec{k}_2 \) \( (\vec{k}_2 \text{ and } \vec{k} = \vec{k}_1 - \vec{k}_2, \text{respectively}) \). The integration over \( \vec{k}_1 \) \( (\vec{k}_2, \text{respectively}) \) then yields \( n_B \), see Eq. (3). This shows that \( \tau_{\text{dec}} \sim 1/\sqrt{n_B} \).

In order to implement decoherence, we follow Ref. [9] and assume that the interaction \( H'_{A-A} \) between atoms in system A is weak. Indeed, sympathetic cooling is used precisely when this condition is met and other procedures fail. To quantify this assumption, we observe that in the absence of \( H'_{A-A} \), a suitable basis for \( \rho_A(t) \) is given by the many–body eigenstates \( |M_1\rangle \) of the trap, i.e., of the three–dimensional harmonic oscillator. Here \( M \) denotes the total excitation energy \( M \hbar \nu \). The running index \( j \) labels the degenerate states. We drop the condition \( H'_{A-A} = 0 \), the degeneracy of the states \( |M_1\rangle \) is lifted, and even states belonging to different values \( M \) get mixed. We quantify the condition that the atoms in system A interact weakly by the requirement that the latter mixing is negligible. We diagonalize \( H_A + H'_{A-A} \) and label the resulting eigenstates by \( |M\mu\rangle \), the eigenvalues by \( \varepsilon(M,\mu) \). Here, \( M \) has the same meaning as before, while \( \mu \) is a new running label.

It turns out that for \( H'_{A-A} \) weak, the master equation has a curious feature. To see this, we take the matrix element of Eqs. (8,10) between a state \( \langle M_1\mu_1| \) and a state \( |M_2\mu_2\rangle \). In-
spection shows that the master equation connects the time derivative of \( \langle M_1 \mu_1 | \rho_A(t) | M_2 \mu_2 \rangle \) with the values of \( \langle (M_1 + \alpha) \mu_3 | \rho_A(t) | (M_2 + \alpha) \mu_4 \rangle \) with \( \alpha \) defined in Eq. (8). In other words, the master equation takes the form of sets of coupled equations, the equations in each set characterized by a fixed value of \( M_1 - M_2 \). The equations in different sets are not coupled with each other. In this situation, decoherence shows that the matrix elements \( \langle M_1 \mu_1 | \rho_A(t) | M_2 \mu_2 \rangle \) with \( M_1 \neq M_2 \) vanish rapidly, and that it suffices to consider only a single set, containing the diagonal block \( \langle M \mu_1 | \rho_A(t) | M \mu_2 \rangle \). Within this block, we may again use decoherence to argue that of these matrix elements, only the ones with \( \mu_1 = \mu_2 \) survive. This is what we assume from now on.

The ensuing reduction in the number of equations is, of course, enormous: Let the total number of states \( |M_j \rangle \) be \( N \). Then, the number of equations needed to determine \( \rho_A(t) \) is \( N^2 \) while the number remaining after we have used the decoherence argument is just \( N \). However, this number is still too large, and a further simplification of the master equation is needed.

III. MICROCANONICAL AVERAGE

Because of decoherence, the reduced density matrix \( \rho_A \) is diagonal in the basis of states \( | M \mu \rangle \). We now assume, in addition, that for fixed \( M \), all matrix elements of \( \rho_A \) are equal. This ergodicity-assumption seems physically reasonable: We expect the equilibration time of the entire system \( A \) to be much larger than the time it takes to equilibrate states which have (nearly) the same energy. Thus,

\[
\langle M_1 \mu_1 | \rho_A(t) | M_2 \mu_2 \rangle = \frac{p_M(t)}{d(M, N_A)} \delta_{M_1, M_2} \delta_{\mu_1, \mu_2} .
\]

The Kronecker delta’s express decoherence, and \( p_M / d(M, N_A) \) is the common value. We define \( d(M, N_A) \) as the number of levels belonging to fixed \( M \) for a system having \( N_A \) particles. Transforming back to the basis of states \( | M j \rangle \), we see immediately that for fixed \( M \), \( \rho_A(t) \) is diagonal in that basis, too, with diagonal elements \( p_M(t) \). We introduce an
explicit notation for the states \(|M_j\rangle\) in terms of the occupation numbers \(n_{\vec{m}}\) of the single-particle states of the harmonic oscillator. These are subject to the constraints \(\sum_{\vec{m}} n_{\vec{m}} = N_A\) where \(N_A\) is the number of atoms in system \(A\), and \(\sum_{\vec{m}} n_{\vec{m}} e_{\vec{m}} = \bar{M}h\nu\). The states \(|M_j\rangle\) are written explicitly as \(|M\{n_{\vec{m}}\}\rangle\). We observe that the \(p_M\) introduced in Eq. (21) obey the sum rule \(\sum_M p_M = 1\).

Taking the partial trace of the master equation over the states \(|M\{n_{\vec{m}}\}\rangle\) with fixed \(M\) and using Eq. (21), we obtain

\[
\frac{dp_M}{dt} = 2 \sum_{\vec{m} \neq \vec{m}'} \Gamma_{\vec{m},\vec{m}'}^{\vec{m}',\vec{m}'} \times \left( \sum_{M'} \frac{p_{M'}}{d(M', N_A)} \sum_{\vec{\lambda}} \langle M'\{n_{\vec{\lambda}}\}|a_{\vec{m}} a_{\vec{m}'}^\dagger |M\{n_{\vec{\lambda}}\}\rangle \langle M\{n_{\vec{\lambda}}\}|a_{\vec{m}'} a_{\vec{m}}^\dagger |M'\{n_{\vec{\lambda}}\}\rangle - \frac{p_M}{d(M, N_A)} \sum_{\vec{\lambda}} \langle M\{n_{\vec{\lambda}}\}|a_{\vec{m}} a_{\vec{m}'}^\dagger a_{\vec{m}'} a_{\vec{m}}^\dagger |M\{n_{\vec{\lambda}}\}\rangle \right).
\] (22)

We note that both terms on the right-hand side of Eq. (22) vanish unless we have \(\vec{m} = \vec{m}'\) and \(\vec{n} = \vec{n}'\). Moreover, the terms with \(\vec{m} = \vec{n}\) cancel, so the case \(\vec{m} = \vec{n}\) is excluded from the summation. We also note that in the sum over \(M'\), all terms vanish but the one for which we have \(M' = M + \alpha\), with \(\alpha\) defined in Eq. (8). The sum \(\sum_{\vec{\lambda}} \langle M\{n_{\vec{\lambda}}\}\rangle \langle M\{n_{\vec{\lambda}}\}\rangle\) is equal to the projector onto the subspace of states with unperturbed energy \(\bar{M}h\nu\). The operator \(a_{\vec{m}}^\dagger a_{\vec{n}}\) acting upon states with energy \(M'\bar{h}\nu\) can anyway only populate states in this subspace. Therefore, the projector can be replaced by the unit operator. As a result, the term multiplying \(p_{M'}\) in Eq. (22) becomes equal to \(\sum_{\vec{\lambda}} \langle M'\{n_{\vec{\lambda}}\}|a_{\vec{m}}^\dagger a_{\vec{m}'} a_{\vec{m}}^\dagger a_{\vec{m}'} |M'\{n_{\vec{\lambda}}\}\rangle\). Divided by \(d(M', N_A)\), this term is nothing but the mean value of \(n_{\vec{m}} [n_{\vec{m}} + 1]\) taken over the states with fixed \(M'\). We denote this quantity by \(\langle n_{\vec{m}} [n_{\vec{m}} + 1]\rangle_{M + \alpha}\). The same argument is applied to the term in Eq. (22) which multiplies \(p_M\) and yields \(\langle n_{\vec{m}} [n_{\vec{m}} + 1]\rangle_M\). As a result, the master equation takes the form of a rate equation,

\[
\frac{dp_M}{dt} = 2 \sum_{\vec{m} \neq \vec{m}'} \Gamma_{\vec{m},\vec{m}'}^{\vec{m}',\vec{m}'} \left( p_{M + \alpha} \langle n_{\vec{m}} [n_{\vec{m}} + 1]\rangle_{M + \alpha} - p_M \langle n_{\vec{m}} [n_{\vec{m}} + 1]\rangle_M \right).
\] (23)

It is straightforward to check that \(\sum_M dp_M(t)/dt = 0\). In Eq. (23), the rate coefficients \(\Gamma\) and the expectation values of the number operators are input quantities defined in the framework of our model, and the \(p_M\)'s are the unknowns.
For later applications of Eq. (23), it is useful to realize that the expectation values depend only upon the single–particle energies and not on the single–particle wave functions. Therefore, we define

$$\bar{\Gamma}_{j,i} = \sum_{\vec{m} \neq \vec{n}} \Gamma_{\vec{n},\vec{m}} \delta_{\vec{j},\vec{m} \cdot \vec{m}} \bar{\nu}_{\vec{n},\vec{m}}(\vec{m}) \delta_{\vec{j},\vec{m} \cdot \vec{m}}(\vec{m}).$$

(24)

Then, Eq. (23) takes the form

$$\frac{dp_M}{dt} = 2 \sum_{\alpha=-K}^{\min(K,K-\alpha)} \sum_{j=\max(0,-\alpha)}^{K} \bar{\Gamma}_{j,j+\alpha} [p_{M+\alpha} \langle n_{j+\alpha}(n_j+1) \rangle_{M+\alpha} - p_M \langle n_{j+\alpha}(n_j+1) \rangle_M].$$

(25)

It is the advantage of this equation that the rates $\bar{\Gamma}$ can be calculated once and tabulated; the solution of Eq. (25) then requires a smaller number of steps than that of Eq. (23).

To use Eq. (23), it is necessary to assign values to the microcanonical averages $\langle n_{\vec{n}}[n_{\vec{m}} + 1] \rangle_M$. We do so by replacing the microcanonical average by the canonical average, determining the temperature $T(E)$ by the thermodynamic relation

$$\frac{1}{T(E)} = \frac{d}{dE} \kappa \ln d(E, N_A)$$

(26)

where $d(E, N_A)$ is the number of microstates of the Boson system $A$ at energy $E$, a smoothed version of the degeneracy $d(M, N_A)$. The microcanonical averages $\langle n_{\vec{n}}[n_{\vec{m}} + 1] \rangle_M$ and $\langle n_{\vec{m}}[n_{\vec{n}} + 1] \rangle_M$ are then approximated by $n_{\vec{n}}(T(E))[n_{\vec{m}}(T(E)) + 1]$ and $n_{\vec{m}}(T(E))[n_{\vec{n}}(T(E)) + 1]$, respectively, with

$$n_{\vec{m}}(T(E)) = \frac{z(E) \exp[-\beta(E)\bar{\nu}(\vec{m})]}{1 - z(E) \exp[-\beta(E)\bar{\nu}(\vec{m})]},$$

(27)

$\beta(E) = 1/(\kappa T(E))$, and $z(E)$ determined from the total number $N_A$ of particles in system $A$. The approximation neglects possible correlations between the occupation numbers $n_{\vec{n}}$ and $n_{\vec{m}}$ in the states labelled $M$. It is, thus, related to a similar approximation used in Section [IV] where such correlations will be discussed.

To carry out the calculation, we need to determine the (energy–smoothed) number of accessible microstates $d(E, N_A)$ of system $A$. We do so for $H'_{A-A} = 0$. We observe that $M$ may attain very large values, and that the degeneracy $d(M, N_A)$ increases rapidly (nearly
exponentially) with increasing $M$. If, for instance, the trap has 30 bound states and the system $A$ consists of $10^4$ atoms, then $M$ assumes all integers between zero and $3 \cdot 10^5$. The very large degeneracy attained for large values of $M$ causes the level density to increase very strongly with energy. This increase is expected to level off at a point where the majority of Bosons occupies the highest available single–particle level.

We follow Ref. [14] to compute $d(E, N_A)$. The number of accessible microstates is related to the grand canonical partition function $\Xi$ via

$$\Xi \equiv \prod_{j=0}^{K} \left(1 - z e^{-\beta \varepsilon_j}\right)^{-g_j} = \sum_{N_A=0}^{\infty} z^{N_A} \sum_{E} e^{-\beta E} d(E, N_A) ,$$

where $K \bar{\hbar} \nu$ is the energy of the highest single–particle orbital in the harmonic trap, $E$ assumes values $M \bar{\hbar} \nu$, and $z$ denotes the fugacity. The degeneracy of single–particle states with energies $\varepsilon_j = j \hbar \nu$ in the harmonic trap is $g_j = (j+1)(j+2)/2$. We introduce $x \equiv e^{-\beta \hbar \nu}$ and rewrite

$$\Xi = \sum_{N_A=0}^{\infty} z^{N_A} \sum_{M=0}^{\infty} x^M d(M, N_A) .$$

The microcanonical number of states $d(E, N_A)$ can be obtained from Eq. (29) by contour integration,

$$d(E, N_A) = \frac{1}{(2\pi i)^2} \oint dx \oint dz \exp \left[ -F(x, z) \right] ,$$

with

$$F(x, z) = \left( \frac{E}{\hbar \nu} + 1 \right) \ln x + (N_A + 1) \ln z + \sum_{j=0}^{K} g_j \ln \left(1 - z x^j \right) .$$

The integrations in Eq. (30) can be performed using the saddle–point approximation. However, care has to be taken in the regime of Bose–Einstein–Condensation (BEC). We recall that BEC is reached in spherical harmonic traps at condensation temperatures $\kappa T_c \approx 0.94 N_A^{1/3} \hbar \nu$, see e.g. Ref. [15]. For $N_A = 400$ Bosons one thus finds $\kappa T_c \approx 6.9 \hbar \nu$. In the presence of BEC the singularity due to the condensate must be excluded from the
saddle–point approximation \cite{14}. The saddle points of Eq. (30) are difficult to obtain for high energies, i.e., energies beyond the maximum of the curve in Fig. 1 and especially for energies close to \( N_A K \hbar \nu \). In this regime we simply invert the single–particle spectrum and solve the corresponding problem for low energies close to the (now highly degenerate) ground state.

Fig. 1 shows the number of microstates \( d(E, N_A) \) as a function of the total energy \( E \) for a system of \( N_A = 400 \) Bosons in a trap with \( K = 21 \). The function \( d(E, N_A) \) grows exponentially for small energies and reaches a maximum; for energies beyond the maximum the finite total number of single–particle orbitals causes a decrease in \( d(E, N_A) \). The number of accessible microstates is a smooth function of energy. In the numerical computations we tabulate \( \ln d(E, N_A) \) for some energies and use these values for interpolation.

![Graph showing entropy as a function of total energy](image)

**FIG. 1.** Entropy \( \ln d(E, N_A) \) as a function of total energy \( E \) for a system of \( N_A = 400 \) Bosons in a trap with highest single–particle orbital \( K = 21 \).

In concluding this Section, we note that all steps in the derivation leading to Eq. (23) apply equally if system \( A \) consists of Fermions instead of Bosons. This results in the following changes. We replace \( n_{\vec{m}}(T(E))[n_{\vec{m}}(T(E)) + 1] \) everywhere by \( n_{\vec{m}}(T(E))[1 - n_{\vec{m}}(T(E))] \). More–
over, Eq. (27) is replaced by \( n_{\vec{m}}(T(E)) = z(E) \exp[-\beta(E)\varepsilon(\vec{m})]/[1+z(E)\exp[-\beta(E)\varepsilon(\vec{m})]] \).

IV. FACTORIZATION

We turn to a different approximation to the master equation, written in the form of Eqs. (9,10). As in Section III, we assume that \( \rho_A(t) \) is diagonal in the \(|M\mu\rangle \) basis, and that -- for fixed \( M \) -- Eq. (21) applies. We recall the basis \(|M\{n_{\vec{m}}\}\rangle \) introduced in Section III.

We now change the notation, omit the letter \( M \), and impose no further restrictions on the \( n_{\vec{m}} \)'s except for \( \sum_{\vec{m}} n_{\vec{m}} = N_A \). In this basis, the reduced density matrix is diagonal, and the master equation takes the form

\[
\frac{d}{dt} \langle \{n_{\vec{m}}\}|\rho_A(t)|\{n_{\vec{m}}\}\rangle = \sum_{\vec{m} \neq \vec{n}} \Gamma_{\vec{m},\vec{n}}^{\vec{m},\vec{n}} \left( 2\langle \{n_{\vec{m}}\}|a_{\vec{n}}^+ a_{\vec{n}}\rho_A(t) a_{\vec{m}}^+ a_{\vec{m}}|\{n_{\vec{m}}\}\rangle \right.
\]

\[
-\langle \{n_{\vec{m}}\}|a_{\vec{n}}^+ a_{\vec{n}}\rho_A(t) a_{\vec{m}}^+ a_{\vec{m}}|\{n_{\vec{m}}\}\rangle 
\]

\[
-\langle \{n_{\vec{m}}\}|\rho_A(t) a_{\vec{n}}^+ a_{\vec{n}} a_{\vec{m}}^+ a_{\vec{m}}|\{n_{\vec{m}}\}\rangle \right).
\]

The last two terms are equal and combine to \(-2n_{\vec{m}}[n_{\vec{m}} + 1] \langle \{n_{\vec{m}}\}|\rho_A(t)|\{n_{\vec{m}}\}\rangle \). Here, \( n_{\vec{m}} \) and \( n_{\vec{m}} \) denote the values of the occupation numbers for the single–particle states \( \vec{n} \) and \( \vec{m} \), respectively, in the set \( \{n_{\vec{m}}\} \). The first term yields \(+2n_{\vec{m}}[n_{\vec{m}} + 1] \langle \{\ldots(n_{\vec{m}} - 1)\ldots(n_{\vec{m}} + 1)\ldots\}|\rho_A(t)|\{\ldots(n_{\vec{m}} - 1)\ldots(n_{\vec{m}} + 1)\ldots\}\rangle \). The notation indicates how the occupation numbers in the set \( \{n_{\vec{m}}\} \) are modified. The master equation becomes

\[
\frac{d}{dt} \langle \{n_{\vec{m}}\}|\rho_A(t)|\{n_{\vec{m}}\}\rangle = 2 \sum_{\vec{m} \neq \vec{n}} \Gamma_{\vec{m},\vec{n}}^{\vec{m},\vec{n}}
\]

\[
\times \left( n_{\vec{m}}[n_{\vec{m}} + 1] \langle \{\ldots(n_{\vec{m}} - 1)\ldots(n_{\vec{m}} + 1)\ldots\}|\rho_A(t)|\{\ldots(n_{\vec{m}} - 1)\ldots(n_{\vec{m}} + 1)\ldots\}\rangle 
\]

\[
n_{\vec{m}}[n_{\vec{m}} + 1] \langle \{n_{\vec{m}}\}|\rho_A(t)|\{n_{\vec{m}}\}\rangle \right).
\]

We now take a partial trace of Eq. (33), summing over all occupation numbers \( n_{\vec{m}} \) of single–particle states \( \vec{m} \) with \( \vec{m} \neq \vec{m}_0 \), keeping the latter fixed. The corresponding partial trace of \( \rho_A(t) \) is denoted by \( p(n_{\vec{m}_0},t) \). This yields

\[
\frac{d}{dt} p(n_{\vec{m}_0},t) = 2 \sum_{\vec{m} \neq \vec{m}_0} \Gamma_{\vec{m}_0,\vec{m}}^{\vec{m}_0,\vec{m}} \left( \sum_{n_{\vec{m}},n_{\vec{m}}}[n_{\vec{m}} + 1]p(n_{\vec{m}},n_{\vec{m}} - 1,n_{\vec{m}} + 1,t) \right.
\]

\[
\left. \sum_{n_{\vec{m}},n_{\vec{m}}} \right).
\]
\[- \sum_{\vec{m}, \vec{n}} n_{\vec{m}} [n_{\vec{n}} + 1] p(n_{\vec{m}}, n_{\vec{n}}, t) \] \quad \text{(34)}

The quantities \( p(n_{\vec{m}}, n_{\vec{n}}, t) \) are defined as partial traces over \( \rho_A(t) \) excluding the single-particle states labelled \( \vec{m}_0, \vec{m}, \) and \( \vec{n} \). It is easy to see that on the right-hand side of Eq. (34), all terms cancel for which both \( \vec{m} \) and \( \vec{n} \) differ from \( \vec{m}_0 \). As a result, we find

\[
\frac{d}{dt} p(\vec{m}_0, t) = 2 \sum_{\vec{n} \neq \vec{m}_0} \Gamma_{\vec{m}_0, \vec{n}} (n_{\vec{m}_0} \sum_{n_{\vec{m}}} [n_{\vec{m}} + 1] p(n_{\vec{m}}, \vec{n}, t) - [n_{\vec{m}} + 1] n_{\vec{n}} p(n_{\vec{m}}, \vec{n}, t)) + 2 \sum_{\vec{m} \neq \vec{m}_0} \Gamma_{\vec{m}, \vec{m}_0} (n_{\vec{m}_0} + 1) \sum_{n_{\vec{m}}} n_{\vec{m}} p(n_{\vec{m}}, n_{\vec{m}_0} + 1, \vec{n}, t) - n_{\vec{m}_0} \sum_{n_{\vec{m}}} [n_{\vec{m}} + 1] p(n_{\vec{m}}, n_{\vec{m}_0}, \vec{n}, t)). \quad \text{(35)}
\]

Except for the assumptions stated at the beginning of this Section, all our steps have been exact. Unfortunately, the Eqs. (35) are not closed. We close them by introducing a factorization assumption for the partial traces of the reduced density matrix. We write

\[
p(n_{\vec{m}}, n_{\vec{n}}, t) = p(n_{\vec{m}}, t) p(n_{\vec{n}}, t). \quad \text{(36)}
\]

We discuss the implications of this assumption below and first deduce the results. For clarity, we replace the symbols \( p(n_{\vec{m}}, t) \) by \( p_{\vec{m}}(n, t) \). This indicates more clearly that \( p_{\vec{m}}(n, t) \) is the density matrix for the single-particle state \( \vec{m} \) with occupation number \( n \). Eq. (35) takes the form

\[
\frac{d}{dt} p_{\vec{m}_0}(n, t) = 2 \sum_{\vec{n} \neq \vec{m}_0} \Gamma_{\vec{m}_0, \vec{n}} (n \sum_{n'} [n' + 1] p_{\vec{m}_0}(n - 1, t) p_{\vec{n}}(n', t) - [n + 1] n' p_{\vec{m}_0}(n, t) p_{\vec{n}}(n', t)) + 2 \sum_{\vec{m} \neq \vec{m}_0} \Gamma_{\vec{m}, \vec{m}_0} (n + 1) \sum_{n'} n' p_{\vec{m}_0}(n + 1, t) p_{\vec{m}}(n', t - 1, t) - n \sum_{n'} [n' + 1] p_{\vec{m}_0}(n, t) p_{\vec{m}}(n', t)). \quad \text{(37)}
\]

Summing Eq. (37) over all \( n \), we obtain \( \frac{d}{dt} \sum_n p_{\vec{m}_0}(n, t) = 0 \). Because we have \( \sum_n p_{\vec{m}_0}(n, t) = \text{tr} \rho_A(t) \), this result is in keeping with the condition \( \text{tr} \rho_A(t) = 1 \). We define the average occupation numbers \( N_{\vec{m}}(t) \) in the single-particle state \( \vec{m} \) at time \( t \) by
\[ N_{\vec{m}}(t) = \sum_n n \ p_{\vec{m}_0}(n,t) . \] (38)

Multiplying Eq. (37) by \( n \) and summing over \( n \), we obtain the following closed system of rate equations for the \( N_{\vec{m}}(t) \),

\[
\begin{align*}
\frac{d}{dt}N_{\vec{m}_0}(t) &= 2 \sum_{\vec{n} \neq \vec{m}_0} \Gamma_{\vec{n},\vec{m}_0}^{\vec{m}} N_{\vec{n}}(t) (N_{\vec{m}_0}(t) + 1) \\
&\quad - 2 \sum_{\vec{m} \neq \vec{m}_0} \Gamma_{\vec{m}_0,\vec{m}}^{\vec{m}} (N_{\vec{m}}(t) + 1) N_{\vec{m}_0}(t) .
\end{align*}
\] (39)

Eq. (39) constitutes the central result of this Section. It is a set of rate equations for the mean occupation numbers \( N_{\vec{n}}(t) \). The form of these equations is intuitively obvious and might even have been written down without much derivation. It is straightforward to check that Eq. (39) implies the condition \( d \sum_n N_{\vec{n}}(t)/dt = 0 \). Thus, the average particle number is conserved.

The rate equations (39) have been derived under the tacit assumption that a finite number of levels in the harmonic–oscillator potential of the trap is available for occupation by atoms in system \( A \). In actual fact, the trap is open, and atoms with energies above a critical energy are able to escape. This fact can most easily be incorporated into Eq. (39) by restricting the values of \( \vec{m}, \vec{n} \) and \( \vec{m}_0 \) to the bound states of the trap, and by adding on the right–hand side of Eq. (39) a loss term. This term allows for scattering into virtual harmonic–oscillator levels which are actually unbound and from which the atoms can escape.

The derivation of the modified form of Eq. (39) is straightforward and yields

\[
\begin{align*}
\frac{d}{dt}N_{\vec{m}_0}(t) &= 2 \sum_{\vec{n} \neq \vec{m}_0} \Gamma_{\vec{n},\vec{m}_0}^{\vec{m}} N_{\vec{n}}(t) (N_{\vec{m}_0}(t) + 1) \\
&\quad - 2 \sum_{\vec{m} \neq \vec{m}_0} \Gamma_{\vec{m}_0,\vec{m}}^{\vec{m}} (N_{\vec{m}}(t) + 1) N_{\vec{m}_0}(t) \\
&\quad - 2 \sum_{\vec{m}' \neq \vec{m}_0} \Gamma_{\vec{m}_0,\vec{m}'}^{\vec{m}'} N_{\vec{m}_0}(t) .
\end{align*}
\] (40)

The summation over \( \vec{m}' \) extends over the virtual states.

The rate coefficients obey the important thermodynamic identity

\[
\Gamma_{\vec{n},\vec{m}}^{\vec{m},\vec{n}} = \Gamma_{\vec{m},\vec{n}}^{\vec{n},\vec{m}} \cdot \exp[-\beta_B (\varepsilon_{\vec{m}} - \varepsilon_{\vec{n}})] .
\] (41)
This follows immediately from the definition in Eq. (7). For the time–independent equilibrium solutions \( N_{m}^{eq} \) of Eq. (39), Eq. (41) implies the values

\[
N_{m}^{eq} = \frac{z_{A} \exp[-\beta_{B} \varepsilon_{m}]}{1 - z_{A} \exp[-\beta_{B} \varepsilon_{m}]},
\]

(42)

with the fugacity \( z_{A} \) determined from the condition \( \sum_{m} N_{m}^{eq} = N_{A} \).

It goes without saying that a parallel derivation applies if the atoms in system \( A \) are Fermions. The final rate equations are obtained by replacing on the right–hand side of Eq. (39) the terms \( (N_{m_{0}}(t) + 1) \) and \( (N_{\bar{m}}(t) + 1) \) by \( (1 - N_{m_{0}(t)}) \) and \( (1 - N_{\bar{m}}(t)) \), respectively. The equilibrium distribution is given by Eq. (42) with the minus sign in the denominator replaced by a plus sign.

The central approximation Eq. (36) assumes that there are no correlations between the occupancies of the states \( m \) and \( \bar{n} \). The one correlation which must exist is total particle number conservation. Thus, we expect that the approximation Eq. (36) may fail whenever \( N_{m} \) or \( N_{\bar{n}} \) approach \( N_{A} \), the total number of particles in system \( A \). For Fermions, this can never happen. Thus, we focus attention on the case of Bosons. A critical situation arises if the number \( n_{0} \) of Bosons in the ground state is comparable to \( N_{A} \). A modification of our previous derivation is, therefore, necessary only for those terms in the master equation which contain the functions \( p(n_{0}, n_{\bar{n}}, t) \). For these terms, we have previously assumed that \( \sum_{n} n p(n_{0}, n_{\bar{n}}, t) = N_{\bar{n}}(t) p(n_{0}, t) \) with \( N_{\bar{n}}(t) \) independent of \( n_{0} \). We now improve on this approximation by letting \( N_{\bar{n}}(t) \) depend on \( n_{0} \). This is accomplished by writing

\[
\sum_{n} n p(n_{0}, n_{\bar{n}}, t) = N_{\bar{n}}(n_{0}, t) p(n_{0}, t)
\]

and by using for \( N_{\bar{n}}(n_{0}, t) \) the ansatz

\[
N_{\bar{n}}(n_{0}, t) = \frac{N_{A} - n_{0}}{N_{A} - N_{0}(t)} N_{\bar{n}}(t),
\]

(43)

with \( N_{0}(t) = \sum_{n_{0}} n_{0} p(n_{0}, t) \) and \( N_{\bar{n}}(t) \) independent of \( n_{0} \). This approximation conserves particle number. It leads to the following modification of the rate equations. We define the variance \( \delta N_{0}^{2} = \sum_{n_{0}} (n_{0})^{2} p(n_{0}, t) - (\sum_{n_{0}} n_{0} p(n_{0}, t))^{2} \) and have, omitting loss terms, for \( \bar{m}_{0} \neq 0 \)

\[
\frac{d}{dt} N_{\bar{m}_{0}}(t) = 2 \sum_{\bar{n} \neq \bar{m}_{0}, 0} \Gamma_{\bar{n}, \bar{m}_{0}}^{\bar{m}_{0}, \bar{n}} N_{\bar{n}}(t)(N_{\bar{m}_{0}}(t) + 1)
\]

17
\begin{align}
-2 \sum_{\vec{m} \neq \vec{m}_0, 0} \Gamma_{\vec{m}_0, \vec{m}} (N_{\vec{m}}(t) + 1) N_{\vec{m}_0}(t) \\
+ 2 \Gamma_{0, \vec{m}_0}^0 N_0(t) \left( N_{\vec{m}_0}(t) \left( 1 - \frac{\delta N_0^2}{N_0(t)(N_A - N_0(t))} \right) + 1 \right) \\
- 2 \Gamma_{\vec{m}_0, 0}^0 N_{\vec{m}_0}(t) \left( N_0(t) \left( 1 - \frac{\delta N_0^2}{N_0(t)(N_A - N_0(t))} \right) + 1 \right). \tag{44}
\end{align}

The equation for $N_0(t)$ has the form
\begin{align}
\frac{d}{dt} N_0(t) &= + 2 \sum_{\vec{n} \neq 0} \Gamma_{0, \vec{n}}^0 N_{\vec{n}}(t) \left( N_0(t) \left( 1 - \frac{\delta N_0^2}{N_0(t)(N_A - N_0(t))} \right) + 1 \right) \\
- 2 \sum_{\vec{n} \neq 0} \Gamma_{0, \vec{n}}^0 N_0(t) \left( N_{\vec{n}}(t) \left( 1 - \frac{\delta N_0^2}{N_0(t)(N_A - N_0(t))} \right) + 1 \right). \tag{45}
\end{align}

Comparing Eqs. (44,45) with the original rate equations (33), we note the appearance of the correction term $\delta N_0^2/(N_0(t)(N_A - N_0(t)))$. This term effectively reduces the coupling between the atoms in the ground state and the rest of the gas and is expected to increase the cooling time. Eqs. (44,45) are not closed as they stand and require the solution of equations for higher moments of the occupation numbers. These, in turn, would not be closed. We address this problem in Eq. (46) below. First, we present a simple estimate of the correction term. We expect the term to be small both for $N_0(t) \ll N_A$ and for $N_A - N_0(t) \ll N_A$. Thus, the correction term should attain its maximum at or near $N_0(t) \approx (1/2)N_A$. It is then reasonable to approximate the correction term by a simple smooth function of $x = N_0/N_A$ in the interval $[0, 1]$, with very small values at the end points and a maximum near the middle. Qualitative support for this idea comes from Figures 1, 2, and 8 of Ref. [13]. Using these Figures, we are led to the conclusion that the correction term does indeed approximately have the form just suggested, with a maximum value of the order of 1 per cent. It must be stressed, of course, that Ref. [13] deals with equilibrium phenomena and not, as we do here, with equilibration processes.

A quantitative evaluation of the correlation requires additional work. To be brief, we only sketch the derivation of the coupled equations which determine both, the mean occupation numbers $N_{\vec{m}}(t)$ and the ground–state correlators. A simple derivation consists in multiplying the master equation, Eqs. (1,2), either with $a_i^\dagger a_j^\dagger$ or with $a_i^\dagger a_j^\dagger a_k^\dagger a_l^\dagger$ and taking the trace.
We use the assumptions introduced above. In particular, we assume that \( \text{tr} \left( a_i^\dagger a_j \rho_A \right) \) and \( \text{tr} \left( a_i^\dagger a_j a_k^\dagger a_l \rho_A \right) \) are diagonal, and that the same assumption applies to the terms involving six creation and annihilation operators. Such terms result from the right–hand side of Eq. (10). For \( \vec{k} \neq 0 \), we define the correlator \( \delta_{\vec{k}} \) by writing \( \text{tr} \left( a_0^\dagger a_0 a_k^\dagger a_0 \rho_A(t) \right) = N_0(t)N_{\vec{k}}(t) + \delta_{\vec{k}}(t) \). To obtain a closed set of equations, we use for \( 0 \neq \vec{k} \neq \vec{m} \neq 0 \) the approximation that \( \text{tr} \left( a_0^\dagger a_0 a_k^\dagger a_0 a_k a_0 \rho_A(t) \right) = N_0(t)N_{\vec{k}}(t)N_{\vec{m}}(t) + N_{\vec{k}}(t)\delta_{\vec{m}} + N_{\vec{m}}(t)\delta_{\vec{k}} \). This approximation amounts to the neglect of all correlations not involving the ground state. As a result, we find that Eqs. (44, 45) retain their form, the terms \( -N_0(t)N_{\vec{m}}(t)\delta N_0^2/ (N_0(t)(N_A - N_0(t))) \) and \( -N_0(t)N_{\vec{m}}(t)\delta N_0^2/ (N_0(t)(N_A - N_0(t))) \) being replaced by \( \delta_{\vec{m}} \) and \( \delta_{\vec{m}} \), respectively. While Eqs. (44, 45) suggest that we have to determine a single function \( \delta N_0^2/ (N_0(t)(N_A - N_0(t))) \), the replacement just indicated shows that we must determine a set of functions \( \delta_{\vec{k}} \). The determining equations for \( \delta_{\vec{k}} \) with \( \vec{k} \neq 0 \) read

\[
\frac{d}{dt}\delta_{\vec{k}}(t) = 2 \left( N_{\vec{k}}(t) + 1 \right) \left( \sum_{\vec{m} \neq \vec{k}, 0} \Gamma_{\vec{k},\vec{m}} \delta_{\vec{m}} \right) + 2\delta_{\vec{k}} \left( \sum_{\vec{m} \neq \vec{k}, 0} \left( \Gamma_{\vec{k},\vec{m}} + \Gamma_{0,\vec{m}} \right) N_{\vec{m}}(t) \right) \\
-2N_{\vec{k}}(t) \left( \sum_{\vec{m} \neq \vec{k}, 0} \Gamma_{\vec{k},\vec{m}} \delta_{\vec{m}} \right) - 2\delta_{\vec{k}} \left( \sum_{\vec{m} \neq \vec{k}, 0} \left( \Gamma_{\vec{k},\vec{m}} + \Gamma_{0,\vec{m}} \right) [N_{\vec{m}}(t) + 1] \right) \\
+2 \left( N_0(t) - N_{\vec{k}}(t) \right) \left( \Gamma_{\vec{k},0} - \Gamma_{0,\vec{k}} \right) [\delta_{\vec{k}} + N_0(t)N_{\vec{k}}(t)] .
\]

The last term in Eq. (46) is the “feeding term”: For \( N_0(t) = 0 \), the homogeneous equation has the solution \( \delta_{\vec{k}}(t) = 0 \). Deviations are due to non–zero occupation numbers of the ground state.

V. CONSISTENCY

In Refs. [11][13], the probability distribution for the ground–state occupation for a system of Bosons coupled to a heat bath was derived for the first time. In this Section, we show that our rate equations yield the same solution, although the system under consideration differs from that of Refs. [11][13]. This result then serves as consistency check for our derivation. Our assumptions are similar to those used in Refs. [11][13]. More specifically, we assume
that the excited levels of system $A$ are in thermal equilibrium with the heat bath (system $B$). This assumption is quantified below.

We specialize Eq. (35) to $\vec{m}_0 = 0$,

$$
\frac{d}{dt} p_0(n, t) = 2 \sum_{\vec{n} \neq 0} \Gamma_{\vec{n}, 0}^{\vec{n}, 0} \left( n p_0(n - 1, t) \langle N_{\vec{n}}(t) \rangle_n - [n + 1] p_0(n, t) \langle N_{\vec{n}}(t) \rangle_n \right) 
+ 2 \sum_{\vec{m} \neq 0} \Gamma_{\vec{m}, 0}^{\vec{m}, 0} \left( [n + 1] p_0(n + 1, t) \langle N_{\vec{m}}(t) \rangle_{n+1} + 1 \right)
- n p_0(n, t) \langle N_{\vec{m}}(t) \rangle_n + 1 \right).
$$

(47)

Here, $\langle N_{\vec{n}}(t) \rangle_n = \sum_{n_B} n_B p(n_B, n_{\vec{n}}, t)/p_0(n, t)$ is the expected value of $N_{\vec{n}}(t)$, given that there are $n$ Bosons in the ground state. We define the cooling and heating coefficients

$$
K_n = 2 \sum_{\vec{n} \neq 0} \Gamma_{\vec{n}, 0}^{\vec{n}, 0} \langle N_{\vec{n}}(t) \rangle_n, \quad H_n = 2 \sum_{\vec{m} \neq 0} \Gamma_{\vec{m}, 0}^{\vec{m}, 0} \langle N_{\vec{m}}(t) \rangle_{n+1} + 1 .
$$

(48)

This yields

$$
\frac{dp_0(n)}{dt} = -\left\{ K_n (n + 1)p_0(n) - K_{n+1} np_0(n - 1)
+ H_n np_0(n) - H_{n+1} (n + 1)p_0(n + 1) \right\}.
$$

(49)

Eqs. (48,49) agree formally with Eq. (8) and the definitions following it of Ref. [11], and with Eqs. (20,21,22) of Ref. [13].

The equilibrium solution of Eq. (49) has the form

$$
p_0(n) = p_0(0) \prod_{i=1}^{n} K_{i-1}/H_i.
$$

(50)

Using this result for all $n = 0, \ldots, N_A$ and the constraint $\sum_{n_{\vec{n}}=0}^{N_A} n p_0(n) = n_0$, we find for the normalization factor

$$
p_0(0)^{-1} = Z = \frac{1}{n_0} \sum_{i=0}^{N_A} i \prod_{j=1}^{i} K_{j-1}/H_j
$$

(51)

where $Z$ is the partition function.

We now assume that for $\vec{n} \neq 0$, the equilibrium mean occupation numbers $\langle N_{\vec{n}} \rangle_n$ are given by a thermal distribution,
\[ \langle N_{\vec{r}} \rangle_n = \frac{z_n \exp[-\beta_B \varepsilon_{\vec{r}}]}{1 - z_n \exp[-\beta_B \varepsilon_{\vec{r}}]} . \]  

(52)

The fugacities \( z_n \) are determined by the condition

\[ \sum_{\vec{r} \neq 0} \langle N_{\vec{r}} \rangle_n = N_A - n . \]  

(53)

We use Eq. (52) and the thermodynamic identity Eq. (41) and find that \( H_n \) can be written in the form

\[ H_n = \exp[\beta_B \varepsilon_0] 2 \sum_{\vec{r} \neq 0} \Gamma_{\vec{r}, 0}^{0, \vec{r}} \langle N_{\vec{r}}(t) \rangle_n / z_n . \]  

(54)

We assume that the temperature \( T_B \) of the heat bath is so low that \( z_n \exp[-\beta_B \varepsilon_{\vec{r}}] \ll 1 \). Then, \( H_n = H \) becomes independent of \( n \), and the normalization condition Eq. (53) implies that \( z_n \) is approximately given by \( z_n = (N_A - n)z \). The constant \( z \) depends upon temperature but is independent of \( n \). Together with Eq. (54) and the definition (48), this yields \( K_n = (N_A - n)Hz \exp[\beta_B \varepsilon_0] \). Inserting this into Eq. (51) and using the normalization condition (51), we find

\[ p_0(n) = \frac{1}{Z} \frac{(z \exp[\beta_B \varepsilon_0])^n}{(N_A - n)!} , \]  

(55)

with

\[ Z = \frac{1}{n_0} \sum_{n=0}^{N_A} \frac{n \exp[\beta_B \varepsilon_0]^n}{(N_A - n)!} . \]  

(56)

The dependence of this result on \( n \) coincides with that of the last displayed equation on the left–hand side of page 023609 of Ref. [13]. This shows the consistency of our result.

VI. RATE COEFFICIENTS

We turn to the computation of the rate coefficients defined in Eq. (4); various quantities used in this equation are in turn defined in Eqs. (2) to (6) and Eq. (8). In what follows we assume that the bath particles can accurately be described by a Boltzmann distribution, see Eq. (3). This assumption simplifies the computation of the rate coefficients considerably.
since it leads to a factorization of the integrals involved. Furthermore, it allows us to approximate in Eq. (7) the factor \([n(k') + 1]\) by unity since the occupation numbers of the bath states are small. We note that the \(\tau\)-integration in Eq. (7) yields a \(\delta\)-function and thus implies \(\varepsilon(k) - \varepsilon(k') + \alpha \hbar \nu = 0\). We may therefore replace in Eq. (2) \(\varepsilon(k)\) by \((\varepsilon(k) + \varepsilon(k') - \alpha \hbar \nu)/2\). We obtain an integrand that is more symmetric in \(k\) and \(k'\). Our starting point is thus

\[
\Gamma_{\vec{m}',\vec{n}'}^{\vec{m},\vec{n}} = \frac{n_B \Lambda_B}{2\hbar^2} e^{+\frac{1}{2} \beta_B \alpha \hbar \nu} \int_{-\infty}^{\infty} \int d^3 k d^3 k' \gamma_{\vec{m}',\vec{n}'}(\vec{k}, \vec{k}') \gamma_{\vec{m},\vec{n}}(\vec{k}', \vec{k})\]

\[
\times \exp \left[ -\beta_B (\varepsilon(k) + \varepsilon(k'))/2 \right] \exp \left[ i (\varepsilon(k) - \varepsilon(k') + \alpha \hbar \nu) \frac{\tau}{\hbar} \right].
\]  

(57)

We introduce the oscillator length \(l_0 = \left(\frac{\hbar}{m \nu}\right)^{1/2}\) and the dimensionless integration variables \(\vec{\kappa} = l_0 \vec{k}, \vec{\kappa}' = l_0 \vec{k}', \vec{\rho} = \vec{x}/l_0, \vec{\rho}' = \vec{x}'/l_0\), and \(t = \tau \nu \frac{\hbar}{m M}\). We also define the dimensionless parameters \(\alpha' = \alpha \frac{M}{m}\) and \(\delta = \frac{m}{M} \beta_B \hbar \nu\). Furthermore, we introduce dimensionless oscillator wave functions without changing our notation. Choosing Cartesian coordinates for positions \(\vec{\rho}, \vec{\rho}'\) and momenta \(\vec{\kappa}, \vec{\kappa}'\) leads to a factorization of the integrals,

\[
\Gamma_{\vec{m}',\vec{n}'}^{\vec{m},\vec{n}} = \omega e^{\frac{i}{2} \alpha' \delta} \int_{-\infty}^{\infty} dt \exp \left( i \alpha' t \right) \prod_{j=x,y,z} I_{m_j, n_j}(t) .
\]  

(58)

The \(t\)-dependent integrals \(I_{m,n}(t)\) are given by

\[
I_{m,n}(t) = \int_{-\infty}^{\infty} dr dr' d\kappa d\kappa' \psi_m(r) \psi_n(r') \psi_m(r') \psi_n(r') \exp \left[ -\frac{\delta}{4} (\kappa^2 + \kappa'^2) \right] \exp \left[ i \frac{t}{2} (\kappa^2 - \kappa'^2) \right] \exp \left[ -i (\kappa - \kappa')(r - r') \right].
\]  

(59)

The normalization factor \(\omega\) in Eq. (58) is given by

\[
\omega = \frac{1}{32 \pi^4} \Lambda_B^3 n_B \alpha^2 \left( M + m \right)^2 \frac{\nu}{M m}.
\]  

(60)

Below we find that \(I_{m,n}(t)\) is an even function in \(t\) and symmetric under exchange \(m \leftrightarrow n\). Thus, the rate coefficients (58) obviously fulfill the thermodynamic identity (31). Most of the parameter dependence for the rate coefficients is simply contained in the normalization \(\omega\), which obeys \(\omega \ll \nu\) in realistic applications. The nontrivial and interesting parameters are \(\delta\) and \(\alpha'\). Below we discuss how the rate coefficients depend on these parameters.
The four integrations over \( r, r', \kappa, \kappa' \) can be done exactly. We first perform the integrations over \( r, r' \) and then the resulting Gaussian integrations over \( \kappa, \kappa' \) \cite{9}. We find

\[
I_{n,m} = 2\sqrt{\frac{\pi}{\delta}} \sum_{k,l=0}^{\text{min}(m,n)} c_{m,n,l} c_{m,n,k} \frac{\Gamma(m + n - k - l + 1/2)}{(1 + \delta/4 + t^2/\delta)^{m+n-k-l+1/2}},
\]

with coefficients

\[
c_{m,n,l} = \frac{(-1)^l \sqrt{m! n!}}{l! (m-l)! (n-l)!}.
\]

Insertion of these results into Eq. (58) leads to an integral over \( t \) of the form

\[
V_n(\alpha') \equiv \int_{-\infty}^{\infty} dt \frac{e^{i\alpha't}}{(1 + \frac{\delta}{4} + \frac{t^2}{\delta})^{n+1/2}}.
\]

This integral can be done exactly \cite{16}. We find

\[
V_n(\alpha') = 2\sqrt{\frac{\delta}{\pi}} \Gamma(1/2 - n) \left( \frac{-|\alpha'|\delta}{2\sqrt{\delta(1 + \delta/4)}} \right)^n K_n \left( |\alpha'|\sqrt{\delta(1 + \delta/4)} \right).
\]

Here \( K_n(x) \) denotes the modified Bessel function and \( n \) is a positive integer. We also need the value of \( V_n(\alpha') \) for \( \alpha' = 0 \). It is safe to take the limit \( \alpha' \to 0 \) in the equation above. We find

\[
V_n(0) = \sqrt{\pi\delta} \frac{\Gamma(n)}{\Gamma(n + 1/2)} (1 + \delta/4)^{-n}.
\]

The exact integration of \( V_n \) constitutes an improvement over the approximate result given in Ref. \cite{9}. We have reduced the computation of the rate coefficients to a six-fold sum

\[
\Gamma_{n,m}^{\vec{m},\vec{n}} = 8 \left( \frac{\pi}{\delta} \right)^{3/2} \omega e^{\frac{1}{2}n'\delta} \sum_{l_x,k_x=0}^{p_x} \sum_{l_y,k_y=0}^{p_y} \sum_{l_z,k_z=0}^{p_z} \left( \prod_{j=x,y,z} c_{m_j,n_j,l_j} c_{m_j,n_j,k_j} \Gamma(q_j + 1/2) \right) V_{1+q_x+q_y+q_z}.
\]

However, the numerical computation of the rate coefficients still presents a formidable problem. This is due to the cancellations that occur in the sum in Eq. (66). These cancellations arise already in the two–fold sum in Eq. (61). For \( \text{min}(m, n) \) exceeding \( \approx 20 \), the individual
terms of the sum vary by so many orders of magnitude that a numerical computation with double precision floating point variables leads to a total loss of precision in the final numerical result. Resorting to extended numerical precision is no practical solution since it increases the computation time by orders of magnitude. Such an increase is unaffordable in view of the fact that realistically, traps contain bound states of to the 30th harmonic–oscillator level or so. The number of rate coefficients needed in such a case is about \( [(1/6) \cdot 30^3]^2/2 \approx 10^7 \).

To circumvent this problem we go back to Eq. (59) and perform the Gaussian integrals over \( \kappa \) and \( \kappa' \) first. This yields

\[
I_{m,n} = 2\pi \sqrt{\frac{2\gamma}{\delta}} \int_{-\infty}^{\infty} dr \psi_n(r) \left( \int_{-\infty}^{\infty} dr' \psi_m(r') \exp \left[ -\gamma (r - r')^2 \right] \psi_n(r') \right) \psi_m(r). \tag{67}
\]

We have used the shorthand notation

\[
\gamma = 2\delta/(\delta^2 + 4t^2). \tag{68}
\]

The integral in Eq. (67) can be viewed as the matrix element of the Gaussian two–body “interaction potential” \( G = \exp \left[ -\gamma (r - r')^2 \right] \) taken between a pair of two–body states, i.e.,

\[
I_{m,n} = 2\pi \sqrt{\frac{2\gamma}{\delta}} \langle \mu | G | \nu \rangle. \tag{69}
\]

We have denoted the states by their quantum numbers as \( \mu = (n, m) \) and \( \nu = (m, n) \). We recall that we are particularly interested in the values of these matrix elements for large values of the integers \( m, n \gg 1 \). In the limit of large quantum numbers a semiclassical evaluation of the matrix element is promising. Following Ref. [17] we use the semiclassical approximation and obtain

\[
\langle \mu | G | \nu \rangle \approx \frac{1}{(2\pi)^2} \int_0^{2\pi} d\vartheta \int_0^{2\pi} d\vartheta' \ e^{-i(\mu - \nu) \cdot \vec{\vartheta}} G \left( \vartheta, \frac{\vec{J}_\mu + \vec{J}_\nu}{2} \right). \tag{70}
\]

Here, \( \vec{J}_\vartheta = \vartheta \) and \( \vec{J}_\mu = \mu \) denote the vectors \((J, J')\) of classical actions \( J \) of the corresponding initial and final quantum states, respectively, and \( \vartheta = (\vartheta, \vartheta') \). We use the harmonic–oscillator relations \( r = \sqrt{2J}\cos \vartheta, \ r' = \sqrt{2J'}\cos \vartheta' \) between positions and angle–action variables and obtain
\[ \langle \vec{\mu}|G|\vec{\nu} \rangle = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\vartheta \int_0^{2\pi} d\vartheta' e^{-i(n-m)(\vartheta-\vartheta')} e^{-\gamma(n+m)(\cos \vartheta - \cos \vartheta')^2}. \]  

Transformation to coordinates \( \phi = \vartheta - \vartheta', \phi' = (\vartheta + \vartheta')/2 \) allows us to perform one integration analytically \([10]\). We arrive at

\[ \langle \vec{\mu}|G|\vec{\nu} \rangle = \frac{1}{\pi} \int_0^\pi d\phi e^{-2\gamma(n+m)\sin^2 \frac{\phi}{2}} I_0 \left( 2\gamma(n + m) \sin^2 \frac{\phi}{2} \right) \cos [(n - m)\phi]. \]

Here \( I_0 \) denotes the modified Bessel function of zeroth order. For the computation of the rate coefficients we perform the remaining integration over \( \phi \) and, subsequently, the integration over \( t \), numerically.

Using Mathematica we checked that for \( m, n \gg 1 \), Eqs. (69) and (72) are in excellent agreement with Eq. (21). This is exactly the regime we are interested in. As expected, the semiclassical approximation becomes inaccurate for \( |m - n| \approx m + n \). This is of no concern to us, however, since our exact expressions (71) and (66) are easily computed numerically in this regime. We conclude that our results permit us to compute the rate coefficients efficiently and accurately for rather large systems.

Fig. 4 shows the rate coefficients for \(^{23}\)Na atoms in an \(^{87}\)Rb bath at temperature \( 1/\beta_B = 7\hbar\nu \) as a function of the energy transfer \( (\varepsilon(\vec{m}) - \varepsilon(\vec{n}))/\hbar\nu \). The plotted line is the average value and the error bars indicate maximal and minimal rate coefficients at given energy transfer. In this example we choose the highest single–particle orbit at excitation energy \( K\hbar\nu \) with \( K = 21 \). The rate coefficients attain maximum values close to zero energy transfer. This fact supports the approximation introduced in Eq. (21). We note that the distribution of the rate coefficients at fixed energy transfer displays a large variance. The number of individual rate coefficients increases dramatically with decreasing modulus of energy transfer. The asymmetry between transitions with negative energy transfer (cooling) and positive energy transfer (heating) is due to the thermodynamic identity (11). Approximately 2\% of the rate coefficients had to be computed using the semiclassical method. This fraction increases with increasing trap cutoff \( K \).
FIG. 2. Distribution of scaled rate coefficients $\Gamma_{\vec{m},\vec{n}}/\omega$ for $^{23}$Na atoms in a $^{87}$Rb bath at temperature $1/\beta_B = 7\hbar\nu$ as a function of energy transfer $(\varepsilon(\vec{m}) - \varepsilon(\vec{n}))/\hbar\nu$: Average value (line), maximal and minimal values (error bars).

For applications of our results, the dependence of the cooling rate on the system parameters is of central interest. The main dependence of the rate coefficients on the system parameters is given by the common factor $\omega$ defined in Eq. (60). This quantity sets the overall time scale. As expected, $\omega$ is linear in both the density of bath atoms and the oscillator frequency and quadratic in the scattering length. It is a symmetric function of the masses of the atoms in systems $A$ and $B$, attaining maximum values when one of the two masses is much larger than the other. The dependence of the rate coefficients on the parameters $\delta = (m/M)\beta_B\hbar\nu$ and $\alpha' = (M/m)\alpha$ is implicit. Eq. (58) expresses the rate coefficients as Fourier transforms with respect to $t$ of a three-fold product of functions $I_{m,n}$. These functions, given in Eq. (61) and (for the semiclassical approximation) in Eq. (69) and Eq. (72), depend on $t$ and on the parameter $\delta$. We note that $I_{m,n}$ is an even function of $t$; we restrict the discussion to non-negative arguments. We found that the $I_{m,n}$’s are positive and
monotonically decreasing functions of $t$ which vanish asymptotically for $t \to \infty$. For fixed $\delta$ and fixed sum $m + n$ the functions $I_{m,n}$ increase with decreasing $|m - n|$. This behavior is unaffected by the integration over $t$ and is clearly reflected in Fig. 2. For fixed $\delta$ and fixed energy transfer $|m - n|$ but increasing values of $m + n$, the values of the functions $I_{m,n}$ increase at the origin but fall off more quickly with increasing $t$. In realistic applications we have $\beta_B \hbar \nu \ll 1$, and this results in $\delta \ll 1$ unless $m \gg M$. For fixed $m, n$, the function $I_{m,n}$ increases with decreasing $\delta$. However, this increase does not translate directly into an increase of the rate coefficients. For large energy transfer $|m - n|$ the increase is over–compensated by the highly oscillating exponential in the integrating over $t$, and the cooling process evolves mainly over transitions to levels that are close in energy. We also observe that an increase of the ration $M/m$ decreases $\delta$ but increases $\alpha'$ and, thus, the frequency of the oscillations of the exponential.

We computed the distribution of rate coefficients also for a system of $^{87}$Rb atoms in a bath of $^{87}$Rb atoms at temperature $1/\beta_B = 7\hbar \nu$. (One may assume that system and bath atoms are in different hyperfine states.) When comparing the distribution to the case of $^{23}$Na atoms in a $^{87}$Rb bath depicted in Fig. 2 we find the following: At small energy transfer the Rb-Rb distribution has average and maximal values that are about three times smaller than for Na-Rb. However, the averages and maximal values of the Rb-Rb system decrease less fast with increasing modulus of the energy transfer and are similar to those of Na-Rb at maximal energy transfer.

**VII. NUMERICAL RESULTS**

In this Section we study the cooling process for Bosons by solving the rate equations (25) and (39) numerically. We compare the results. As an example we take system $A$ to be composed of $N_A = 400$ $^{23}$Na atoms, while the $^{87}$Rb bath has the temperature $1/\beta_B = 7\hbar \nu$. This temperature is slightly above the condensation temperature $\kappa T_c = 6.93\hbar \nu$ for harmonic traps. We assume that the highest bound state in the harmonic trap has energy $K\hbar \nu$ where
\[ K = 21. \]

In the microcanonical approach, the rate equations are given by Eq. (25). The computation of the input parameters \( \langle n_j(n_j-\alpha + 1) \rangle_M \) and \( \bar{\Gamma}_{j,i} \) is described in Section \textsection III and Section \textsection VI, respectively. We checked that the computed expectation values \( \langle n_j \rangle_M \) fulfill the sum rules
\[
\sum_j \frac{1}{2}(j + 1)(j + 2) \langle n_j \rangle_M = N_A \quad \text{and} \quad \sum_j \frac{1}{2}j(j + 1)(j + 2) \langle n_j \rangle_M = M
\]
to 1% accuracy. The homogeneous system of linear equations given by Eq. (25) can be put into matrix form. We introduce the sparse matrix \( A \) which has \( 2K + 1 \) non-vanishing elements in each row and column and write Eq. (25) somewhat symbolically as
\[
\frac{dp_M}{dt} = \sum_N A_{M,N} p_N.
\]
We note, however, that in our example the matrix \( A \) has dimension 8401. With \( \max(M - K, 0) \leq N \leq \min(M + K, KN_A) \), the off-diagonal elements of \( A \) are given by
\[
A_{M,N} = 2 \sum_{j=\max(0,M-N)}^{\min(K,K+M-N)} \bar{\Gamma}_{j,j+N-M} \langle n_{j+N-M}(n_j+1) \rangle_N , \tag{73}
\]
and the diagonal elements are
\[
A_{M,M} = -2 \sum_{\alpha=\max(-K,M-KN_A)}^{\min(K,M)} \sum_{j=\max(0,-\alpha)}^{\min(K,K-\alpha)} \bar{\Gamma}_{j,j+\alpha} \langle n_{j+\alpha}(n_j+1) \rangle_M . \tag{74}
\]
The limits on the summations result either from Eq. (24) or are a consequence of the identities \( \langle n_i(n_j+1) \rangle_M = 0 \) for \( i > M \) and \( \langle n_i(n_j+1) \rangle_{K(N_A-1)+l} = 0 \) for \( i < l \). The conservation of probability in Eq. (25) is manifest since the elements in each column of \( A \) sum up to zero. The complete diagonalization of the matrix \( A \) is expensive and unnecessary. Instead, we compute only the eigenvalues with the largest real parts. For stability reasons, there are no eigenvalues with positive real parts. The equilibrium solution is determined by the zero eigenvalue. The equilibration rate is thus equal to the modulus of the real part of the eigenvalue with largest negative real part; the corresponding mode is damped out last. The eigenvalues of interest are computed using the sparse matrix solver ARPACK [18]. Within our numerical accuracy we found one zero eigenvalue and no eigenvalues with positive real parts. For the equilibration rate we found \( \gamma_{eq} \approx 2.7 \times 10^4 \omega \), with \( \omega \) defined in Eq. (60). The equilibrium energy \( E_{eq} = 3961.3 \) can easily be computed from the eigenvector belonging to
eigenvalue zero; alternatively, it can be obtained from the probability distribution for large

times in a numerical integration of the rate equations (25).

It is also interesting to follow the time evolution of the total energy $E(t) = \hbar \nu \sum M p_M(t)$ for a system of Na atoms in a Rb bath. As the initial condition we take $p_{KN_A} = 1$ and vanishing values for all other probabilities. Fig. 3 shows the time evolution of $E(t)$ as obtained upon integration of the rate equations. Initially, the decay is fast but non–exponential. This is due to the fact that many eigenvalues of the matrix $A$ contribute to the cooling process. At later times the equilibrium value $E_{eq}$ is approached exponentially fast with the rate $\gamma_{eq}$ given above. Inspection of the data used in Fig. 3 shows that the temperature corresponding to the equilibrium energy $E_{eq}$ is $\kappa T = 7.0 \hbar \nu$. This agrees well with the temperature of the bath.

![Graph](image)

FIG. 3. Energy difference $E(t) - E_{eq}$ as a function of time within the microcanonical approach in the Na-Rb system.

We turn to the description of the cooling process in terms of the rate equations (39). The number of coupled nonlinear differential equations defined by Eq. (39) is given by the
number of single–particle states in the trap and equals 2024 in our example. Again, we consider Na atoms in a Rb bath. As the initial condition we take the $N_A = 400$ Bosons to be equally distributed over the degenerate single–particle orbitals with energy $K\hbar\nu$ while all other orbitals are empty. This initial condition corresponds to the situation discussed above for the microcanonical approach. Fig. 4 shows a plot of the total energy as a function of time. Initially, the decay is fast but nonexponential and can barely be distinguished from the decay within the microcanonical approach (compare with Fig. 3). At later times the equilibrium $E_{eq} \approx 3901$ is approached exponentially fast with the equilibration rate $\gamma_{eq} = 1.6 \times 10^4 \omega$. This rate was determined from the time evolution shown in Fig. 4. Alternatively, the rate might be obtained upon linearization of the rate equations (39) around the equilibrium solution of Section V. However, we did not pursue this point any further. The equilibrium energy is about 2% smaller than the corresponding value found in the microscopic approach. According to the data used in Fig. 4 we find a temperature of $\kappa T = 6.9\hbar\nu$, slightly deviating from the bath temperature. We recall that the bath temperature enters the rate equations through the rate coefficients. Within our numerical accuracy, and especially because of the semiclassical approximation, we expect the relative error of the rate coefficients to be a few percent. In view of this fact, the agreement between the temperature of the bath and the one found in our calculation, is quite satisfactory.
Comparing the results obtained in the microcanonical approach and by using factorization, we note that the equilibration rate obtained from the microcanonical approach is about a factor $\approx 1.7$ larger than the corresponding rate found using factorization. The loss of energy at short times is, however, practically identical in both approaches. It is evident from Fig. 3 and Fig. 4 that most of the energy is removed from system $A$ during the early period of the cooling process. Therefore, both approaches yield comparable predictions for the cooling time. For example, about 90% of the finally removed energy $E(t = 0) - E_{\text{eq}}$ have been transferred to the bath at a time $t_{\text{cool}} \approx 0.6 \times 10^{-4} \omega^{-1}$.

We also note that the results obtained in the microcanonical approach are somewhat less sensitive to the exact values of the rate coefficients than those obtained using factorization. This is plausible since only sums over many rate coefficients enter the rate equations in the former case.

Let us finally discuss sympathetic cooling of systems with equal masses. Note that the regime of similar masses lies somewhat outside the scope of this work. We recall that
the bath particles are assumed to be much heavier than the particles of the system. This
difference in masses is also reflected by the use of different wave functions for the particles
of the bath and the particles of the system. A detailed computation with identical wave
functions for system and bath may thus yield quantitatively different results. With these
cautious remarks in mind we turn to sympathetic cooling of $^{87}$Rb atoms in a bath of $^{87}$Rb
atoms. (System and bath atoms are assumed to be in different hyperfine states). The results
apply, of course, equally to all other cases where cooled atoms and bath particles have equal
masses. Within the microcanonical approach we found equilibration to a final state with
energy $E_{eq} = 3965.9\hbar\nu$. This corresponds to the temperature $\kappa T = 7.0\hbar\nu$ and agrees well
with the temperature of the bath. The equilibration rate is $\gamma_{eq} = 1.1 \times 10^4 \omega$ and the cooling
time $t_{cool} \approx 1.5 \times 10^{-4} \omega^{-1}$. Using the approach based on factorization we found for the energy
of the equilibrated system $E_{eq} \approx 3900\hbar\nu$ corresponding to a temperature $\kappa T \approx 6.9\hbar\nu$. The
equilibration rate was $\gamma_{eq} \approx 0.6 \times 10^4 \omega$; the cooling time $t_{cool} \approx 1.5 \times 10^{-4} \omega^{-1}$. At the initial
stages of the cooling process there is again barely any difference between the microcanonical
approach and the one based on factorization. Nevertheless, equilibration rates vary by a
factor of about 1.7. Comparing the results for the Rb-Rb system with the Na-Rb system
one thus finds that sympathetic cooling times (in units of $\omega^{-1}$) decrease significantly with
decreasing mass ratio $m/M$ between system and bath particles. In our case, the factor
(about 2.5) is similar to the factor reported at the end of Section VI.

VIII. CONCLUSIONS

We have derived rate equations for the sympathetic cooling of systems composed of
Bosons or of Fermions. The rate equations were obtained from the master equation derived
in Ref. [9] in a sequence of steps. First we used the perturbatively weak interaction $H'_{A-A}$
between the particles in the system to be cooled to lift the degeneracy of the many-body
states in the trap. This allowed us in a second step to use the decoherence argument
and resulted in a reduced density matrix of diagonal form. In a third step we invoked an
ergodicity argument and assumed that the equilibration between (quasi–)degenerate states is much faster than the cooling process; this assumption reduced the number of independent diagonal elements further. From here on we proceeded along two different routes. Within the microcanonical approach we obtained rate equations that govern the occupation probabilities of sets of (quasi–)degenerate many–body states. This results in a linear problem with sparse matrix. The dimension of the problem increases with particle number and trap cutoff. Alternatively, we traced the reduced density matrix over single–particle states. Assuming that occupation probabilities for different orbitals factorize we obtained a nonlinear set of rate equations for the mean occupation probabilities of the single–particle orbitals. The dimension of this problem depends only on the trap cutoff. We showed how to extend this approach to include correlations and particle escape from the open trap, although we did not yet test these extensions numerically.

We provided several checks on our assumptions. To check the consistency of our assumptions we used the rate equations and computed the probability distribution for the ground state occupation; the results agree with those of the literature. We further showed that the decoherence argument is justified. Off–diagonal elements of the reduced density matrix decay on a time scale that is inversely proportional to the square root of the number of bath particles and, thus, very short. The ergodicity argument was supported by the dependence of the rate coefficients on energy transfer, see Fig. 2.

Any solution of the rate equations requires as input the rate coefficients. We derived analytical expressions for these coefficients. A numerical evaluation of the resulting formulas becomes impractical, however, for transitions between high–lying single–particle states that are close in energy. We solved this problem by using a semiclassical approximation. We note that the computation of the rate coefficients is the time–consuming part in practical applications of the rate equations derived in this work. We discussed the dependence of the rate coefficients on the parameters of the system.

The two different rate equations obtained in this paper yield results that are in semi–quantitative agreement. Within both approaches, the cooling times are about the same:
Both descriptions of the cooling process yield almost identical short-time behavior and practically identical final states of the system. The equilibration rates, however, differ by a factor of about 1.6. It is not easy to point to the origin of this difference. We recall that input parameters (rate coefficients) were computed to a relative accuracy of about a few percent. We can only speculate that the long-time behavior of the solutions to the rate equations are sensitive to such details.

In practice, the choice between both approaches depends on the problem under consideration. One has to solve either a large linear problem whose dimension depends on trap cutoff and particle number, or a smaller nonlinear one with a dimension that only depends on the trap cutoff. The treatment of large systems requires the computation of a large number of rate coefficients. Sums of rate coefficients enter the rate equations in the microcanonical approach. Larger systems may become accessible more easily once these sums can be obtained without computing all terms individually. Work along this direction is in progress. Likewise, we have not tested yet the validity of the factorization assumption by solving the combined system of equations, Eqs. (46) and (44, 45).

We have assumed throughout that the interaction $H'_{A-A}$ between particles in the cooled system is weak. It is known [15], however, that no matter how small $H'_{A-A}$ is, this interaction cannot be neglected in the condensed state once the number of condensed atoms is sufficiently large. Does this statement – and the corresponding consideration for the superconducting state of Fermions – seriously limit our approach? We believe not. More precisely: There exists a generalization of our approach which overcomes the problem. It is based on the observation that it is sufficient to deal with the system in mean-field approximation since thermodynamic properties are unaffected by collective excitations [15]. Our rate coefficients are defined in terms of single-particle states and single-particle energies. We may take these as solutions of mean-field equations. Thus, we can extend our scheme as follows. We follow the cooling process as described by our rate equations to the point where the occupation number $n_0$ of the ground state exceeds the critical value at which interactions become important. We define a new set of single-particle wave functions and energies self-
consistently for that value of $n_0$ and calculate the rate coefficients. In this way we may proceed to arbitrarily large values of $n_0$, and similarly for a system of Fermions. Obviously, implementation of this scheme is practical only if we succeed in speeding up the calculation of the rate coefficients or of sums over these coefficients.

The authors are grateful to A. Most and M. Weidemüller for suggesting this problem, and for many stimulating discussions. They also thank S. J. Wang for valuable suggestions. ANS acknowledges support by a fellowship of FAPESP (Fundação de Amparo a Pesquisa do Estado de Sao Paulo). TP thanks the Max–Planck–Institut für Kernphysik, Heidelberg, for its hospitality during the initial stages of this work and acknowledges support as a Wigner Fellow and staff member at the Oak Ridge National Laboratory, managed by UT-Battelle, LLC for the U.S. Department of Energy under Contract DE-AC05-00OR22725.

[1] D. J. Wineland, R. E. Drullinger, and F. L. Walls, Phys. Rev. Lett. 40 (1978) 1639.

[2] R. E. Drullinger, D. J. Wineland, and J. C. Berquist, Appl. Phys. 22 (1980) 365.

[3] D. J. Larson, J. C. Berquist, J. J. Bollinger, W. M. Itano, and D. J. Wineland, Phys. Rev. Lett. 57 (1986) 70.

[4] Atomic Physics 9, edited by R. S. van Dyck, Jr., and E. N. Fortson, World Scientific, Singapore 1985.

[5] A. G. Truscott, K. E. Strecker, W. I. McAlexander, G. B. Partridge, R. G. Hulet, Science 291 (2001) 2570.

[6] F. Schreck, G. Ferrari, K. L. Corwin, J. Cubizolles, L. Khaykovich, M.-O. Mewes, and C. Salomon, Phys. Rev. A 64 (2001) 011402(R).

[7] C. J. Myatt, E. A. Burt, R. W. Ghrist, E. A. Cornell, and C. E. Wieman, Phys. Rev. Lett. 78 (1997) 586.
[8] G. Delannoy, S. G. Murdoch, V. Boyer, V. Josse, P. Bouyer, and A. Aspect, Phys. Rev. A 63 (2001) 051602(R).

[9] M. Lewenstein, J. I. Cirac, and P. Zoller, Phys. Rev. A 51 (1995) 4617.

[10] W. Geist, L. You, and T. A. B. Kennedy, Phys. Rev. A 59 (1999) 1500.

[11] M. O. Scully, Phys. Rev. Lett. 82 (1999) 3927.

[12] J. I. Kim, M. C. Nemes, A. F. R. de Toledo Piza, and H. E. Borges, Phys. Rev. Lett. 77 (1996) 207.

[13] V. V. Kocharovsky, M. O. Scully, S.-Y. Zhu, and M. S. Zubairy, Phys. Rev. A 61 (2000) 023609.

[14] M. Holthaus and E. Kalinowski, Ann. Phys. (N.Y.) 276 (1999) 321.

[15] F. Dalfovo, S. Giorgini, L. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71 (1999) 463.

[16] I. S. Gradshteyn and I. M. Rizhik, Table of Integrals, Series and Products, Academic Press (San Diego 2000).

[17] J. J. Morehead, Phys. Rev. A 53 (1996) 1285.

[18] R. B. Lehoucq, D. C. Sorensen, and C. Yang, ARPACK User’s Guide: Solution to large scale eigenvalue problems with implicitly restarted Arnoldi methods, FORTRAN code available under http://www.caam.rice.edu/software/ARPACK/