Thermalization in mixtures of ultracold gases
Marco Anderlini, David Guery-Odelin

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I. INTRODUCTION

Ultracold mixtures of alkali atoms have attracted great interest among atomic physicists. The ability to simultaneously cool and trap multiple species offers the possibility to study a large variety of physical phenomena not previously accessible with a single species such as novel degenerate quantum systems made of Fermi-Bose mixtures \[1\].

Thermalization plays a crucial role in the cooling of a sample by evaporation, and/or in the implementation of sympathetic cooling. The detailed knowledge of the underlying physics is all the more important for experiments where the time available to perform evaporation is limited \[2\], or for the optimization of the evaporation ramp in the multi-partial-wave regime \[3\]. In addition the return to equilibrium of a gas initially prepared in an out-of-equilibrium state is a widely used way to infer the value of the scattering length \[4, 5, 6, 7, 8, 9, 10\].

The purpose of this paper is to provide a theoretical framework to describe the thermalization between two cold gases confined in a box or a harmonic trap. In contrast to previous theoretical studies on this subject \[2, 4, 11\], we explicitly take into account all partial waves involved in the collision process, and we work out the role played by the confinement in all collisional regimes. Since the basic mechanism described by the Boltzmann equation is binary collisions, two-component systems exhibit all the complexities of \(n\)-component systems. The generalization of the results we obtain to systems containing more than two species is therefore straightforward.

The paper is organized as follows. Section II describes the theoretical framework used to investigate the dynamics of thermalization. Section III is devoted to the simple case of a gas confined in a box. It gives the explicit expression for the rethermalization time including the interference terms between all partial waves involved in the collision process. Section IV addresses the same problem for a gas trapped in an isotropic harmonic trap.

II. THEORETICAL FRAMEWORK

The gas \(i (i = 1, 2)\) consists of \(N_i\) particles of mass \(m_i\) initially thermalized at \(T_i^0\). The dynamics of the gas is described by a set of two coupled Boltzmann equations for each phase-space distribution function \(f_i(\mathbf{r}, \mathbf{v}, t)\):

\[
\frac{\partial f_i}{\partial t} + \{f_i, H_i\} = I_{ii}[f_i] + I_{ij}[f_i, f_j], \quad i \neq j, \quad (1)
\]

The distribution function \(f_i\) for the species \(i\) is governed by the Hamiltonian \(H_i\) through the Poisson bracket \(\{f_i, H_i\}\), and by binary collisions. The appearance of two collision terms on the right-hand side of Eq. (1) is a result of the possibility of \(i\) to change through both self collisions (\(i\)-\(i\) collisions) or cross collisions (1-2). The expression for the collision integrals is

\[
I_{ij}[f_i, f_j] = \int d^2\Omega d^3v_B |\mathbf{v}_B - \mathbf{v}_A| \frac{d\sigma_{ij}}{d\Omega} \times [f_i(\mathbf{r}, \mathbf{v}_A, t)f_j(\mathbf{r}', \mathbf{v}_B', t) - f_i(\mathbf{r}, \mathbf{v}_A, t)f_j(\mathbf{r}, \mathbf{v}_B, t)], \quad (2)
\]

where \(i, j = 1, 2\). They account for elastic collisions between particles labelled \(A\) and \(B\). We denote the velocities of the two atoms before they interact with each other by \(\mathbf{v}_A\) and \(\mathbf{v}_B\), and after the collision by \(\mathbf{v}_A'\) and \(\mathbf{v}_B'\). The expression for the collision terms can be easily extended to include the effects of both Bose and Fermi statistics leading to the Boltzmann-Nordheim equation \[12, 13\]. In fact, most of the results discussed in this paper also hold in the presence of quantum degeneracy, provided the system is not Bose-Einstein condensed. The quantitative estimates of collision effects presented in this work are, however, based on classical statistics. As shown in Refs \[14\] for bosons and \[15\] for fermions, our approach, based on the result of the classical physics, is valid as soon as the temperature of the sample is larger than twice the temperature for degeneracy, i.e. the critical temperature for bosons and the Fermi temperature for fermions.

The collision problem is simplified by an appropriate change of variables. We introduce the center of mass velocity \(\mathbf{v}_0 = (m_A\mathbf{v}_A + m_B\mathbf{v}_B)/(m_A + m_B)\), the total mass
\[ M = m_A + m_B, \] the relative velocity \( \mathbf{v}_r = \mathbf{v}_A - \mathbf{v}_B, \]
and the reduced mass \( \mu = m_A m_B / M. \) The relative velocity changes from the value \( \mathbf{v}_r \) before the collision to the value \( \mathbf{v}_r' \) after the collision, keeping the same value for the modulus \( v_r = v_r' \) because of energy conservation. The collision process is described by specifying the scattering direction with the polar angle \( \theta' \) and the azimuthal angle \( \varphi' \) of the final relative velocity \( \mathbf{v}_r' \) with respect to the initial relative velocity \( \mathbf{v}_r \) before the collision. The corresponding solid angle \( d^2\Omega' = d\varphi' \sin \theta' d\theta' \) enters the expression for the integrand of the collision integrals.

The angular dependence of the elastic scattering directly derives from the partial-waves decomposition of the scattering amplitude in the quantum mechanical description of interactions [14]. For non-identical atoms, the asymptotic form of the scattering amplitude \( f(k, \theta') \) reads

\[
f(k, \theta') = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \epsilon^l \sin(\delta_l) P_l[\cos(\theta')],
\]
where \( k = \mu v_r / \hbar, \theta' \in [0, \pi] \) and \( P_l[\cos(\theta')] \) are the Legendre polynomials. All the complexity of the interatomic potential is contained in the \( k \)-dependence of the phase shifts \( \delta_l \). The differential cross section for non-identical atoms is given by \( d\sigma_{ij}/d\Omega' = |f(k, \theta')|^2 \).

For identical atoms, we have to take into account the (anti)symmetrization principle. Accordingly the differential cross section takes the form:

\[
d\sigma_{ii} = |f(k, \theta') + \epsilon f(k, \pi - \theta')|^2,
\]
where \( \epsilon = 1 \) for bosons and \( \epsilon = -1 \) for fermions. The integration must be carried out only in the half sphere \( \theta' \in [0, \pi/2] \). As a consequence of the parity of the spherical harmonic, the only partial waves contributing to the scattering cross-section for polarized bosons (respectively, fermions) correspond to even (respectively, odd) values of \( l \). The interference between partial waves are contained in the differential cross section [15].

A relevant parameter to describe the thermalization of the gases is the collision rate. The average total number of collisions per unit of time \( \Gamma_i \) for atom species \( i \) and \( j \) is obtained by integrating over space and velocity the output channel term of the collision integral in Eq. [2]:

\[
\Gamma_{ij} = \int d^3r_d^3v_A d^3v_B \sigma_{ij} |\mathbf{v}_A - \mathbf{v}_B| f_i(\mathbf{r}, \mathbf{v}_A, t) f_j(\mathbf{r}, \mathbf{v}_B, t)
\]

From this quantity we deduce the expression for the mean collision rate per atom \( \bar{\Gamma}_{ij} = \Gamma_{ij} / N_i \). The integrated cross section \( \sigma_{ij} \) is just the sum of the contributions from partial-waves:

\[
\sigma_{ij}(v_r) = (1 + \delta_{ij}) \sum_l \frac{4\pi}{k^2} (2l + 1) \sin^2 \delta_l,
\]
where the factor \( (1 + \delta_{ij}) \) accounts for the constructive interference of indistinguishable scattering channels for identical atoms, \( \delta_{ij} \) being the Kronecker delta symbol. The sum in Eq. [3] is taken over even (resp. odd) values for identical \( i = j \) bosons (resp. fermions), and over all integer values for non-identical atoms \( i \neq j \). The expression for the collision rate is just a simple sum over the partial waves, it does not exhibit interference. This is to be contrasted with the expression of the thermalization rate as will be illustrated in the next section.

The determination of the thermalization rate is based on the method of averages [17] combined with an appropriate ansatz. Starting from Eq. [1], one readily derives the equation for the average value of a general dynamical quantity \( \mathcal{O}(\mathbf{r}, \mathbf{v}_i) \):

\[
\frac{d\langle \mathcal{O} \rangle_i}{dt} + \langle \mathcal{O}\{f_i, H_i\}\rangle_i = \langle \mathcal{O}I_i\rangle_i + \langle \mathcal{O}I_{ij}\rangle_i,
\]
where the average is taken in both position and velocity space: \( \langle \mathcal{O}\rangle_i = \int d^3r d^3v_i f_i(\mathbf{r}, \mathbf{v}_i, t) \mathcal{O}(\mathbf{r}, \mathbf{v}_i) / N_i \). As a consequence of the collisional invariants — number of atoms, momentum, and energy —, \( \langle \mathcal{O}I_{ij}\rangle_i = 0 \) if \( \mathcal{O}_i \) is of the form \( \mathcal{O}_i = a(\mathbf{r}) + b(\mathbf{r}) \cdot \mathbf{v}_i + c(\mathbf{r}) \mathbf{v}_i^2 \).

### III. THERMALIZATION IN A BOX

As a first application of the model, we consider the thermalization of a two-species gas in a box of volume \( V \). We assume that atoms can undergo only specular reflection on the walls of the box, which can be realized experimentally by using the dipolar optical force [18]. Initially, the gases are at different temperatures, \( T_i \) and \( T_j \), for the gases of species \( i \) and \( j \), respectively. The Boltzmann dynamics. To evaluate the thermalization time, we write the equation for the mean total kinetic energy \( \langle N_i m_i \mathbf{v}_i^2 / 2 \rangle_i \) of species \( i \):

\[
\frac{d}{dt} \left( \frac{N_i m_i \mathbf{v}_i^2}{2} \right)_i = \left( \frac{N_i m_i \mathbf{v}_i^2}{2} \right)_i \equiv \Sigma_i, \quad j \neq i.
\]

The Poisson bracket of Eq. [4] vanishes for a homogeneous system, and the self collision integral term does not contribute because of conservation of kinetic energy for elastic collisions. The calculation of the collision integral term requires an ansatz for the distribution function. We choose a Gaussian ansatz for the phase-space distribution function of each species:

\[
f_i(\mathbf{v}_i, t) = N_i \exp \left( -\frac{m_i \mathbf{v}_i^2}{2 k_B T_i} \right),
\]

where \( N_i = N_i m_i^{3/2} / (V (2 \pi k_B T_i)^{3/2}) \) is the normalization factor. The time dependence is contained only in the effective temperatures \( T_i \). We assume that \( (T_i^0 - T_f)/T_f \ll 1 \) and \( (T_i^0 - T_f)/T_f \ll 1 \). Consequently, we can evaluate the total number of cross collisions per unit of time by setting \( T_i = T_2 = T_f \) in Eq. [5] with the
Gaussian ansatz for the distribution functions:
\[
\Gamma_{12} = \frac{2}{\sqrt{\pi}} \frac{N_1 N_2}{V} e^{c(\sigma_{12})},
\]  
where we have introduced the velocity \( c = (2k_B T_f/\mu)^{1/2} \) and the thermally averaged cross section \( \langle \sigma_{12} \rangle = 2 \int_0^\infty dx \sigma_{12}(cx)x^2e^{-x^2} \).

The expansion around the final temperature \( T_f \) of the collision terms yields a set of linear equations. We can rewrite them in the form (see Appendix A):
\[
\frac{d(T_i - T_j)}{dt} = -\left( \frac{N_i + N_j}{N_i N_j} \right) \frac{T_i - T_j}{\tau}, \quad i \neq j,
\]  
with
\[
\frac{1}{\tau} = \frac{8\mu}{3M} \langle \sigma_{12} \rangle \Gamma_{12},
\]  
where \( \langle \sigma_{12} \rangle = \int_0^\infty dx \sigma_{12}(cx)x^2e^{-x^2} \). The quantity \( \sigma_{12}(cx) \) is defined as:
\[
\sigma_{12}(cx) = 2\pi \int_0^\pi \sin \theta' (1 - \cos \theta') \frac{d\sigma_{12}}{d\Omega} d\theta'.
\]

The new feature of this expression arises from the interference between partial waves resulting from the angular integration. This is in contrast to the expression for the total cross section, which just contains a simple sum over partial waves. We show in Appendix A, that interference occur only between partial waves differing by at most one unit of angular momentum.

We thus find that the relaxation corresponds to an exponential decay but the thermalization times \( \tau \) is not in general proportional to the collision rate because it contains partial wave interference terms.

At very low temperature where only s-waves contribute to the collision process, no interference can occur and the relaxation time is proportional to the inverse of the collision rate. If the cross section depends on the relative wave vector \( k \) of the collision, the factor of proportionality depends on temperature.

For a cross section of the form \( \sigma_{12}(k) = 4\pi a_{12}^2/(1 + a_{12}^2 k^2) \), one finds
\[
\langle \sigma_{12} \rangle = 4\pi a_{12}^2 \xi[1 - \xi e^\xi \Gamma(0, \xi)],
\]
\[
\langle \sigma_{12} \rangle = 2\pi a_{12}^2 \xi[1 - \xi + \xi^2 e^\xi \Gamma(0, \xi)],
\]
where \( \xi = \hbar^2/(2\mu k_B T_f a_{12}^2) \) and \( \Gamma(a, z) = \int_z^\infty \rho^{a-1}e^{-\rho}d\rho \).

In the very low temperature limit \( \xi \gg 1 \), we have \( \langle \sigma_{12} \rangle = \langle \sigma_{12} \rangle = 4\pi a_{12}^2 \); in the unitary limit \( \xi \ll 1 \), we obtain \( \langle \sigma_{12} \rangle = 2\langle \sigma_{12} \rangle = 2\pi \hbar^2/(\mu k_B T_f) \). As a consequence, the number \( \langle \Gamma_{12} \rangle \) of inter-species collisions per atom required to equilibrate the temperature of a two-component system made of atoms of the same mass varies from 1.5 in the very low temperature limit to 3 in the unitary limit according to Eq. (14).

In the following, we explicitly derive the curves for the thermalization time \( \tau \) and the inter-species collision rate \( \gamma \) for the same number of \( ^{87}\text{Rb} \) atoms \( N_1 = N_2 = N \) in two different internal states \( |5S_{1/2}, F = 2, m = 1 \rangle \) and \( |5S_{1/2}, F = 1, m = -1 \rangle \). This calculation has been performed by taking into account the first five partial wave contributions for the cross collisions [19]. We plot in Fig. (1) the average cross section \( \langle \langle \sigma_{12} \rangle \rangle \) normalized to its value with the cross section taken at zero energy. The resonance shape results from a d-wave resonance, which in turn tends to magnify the interference terms between p-d, and d-f partial waves, leading to a significant difference between the thermalization times calculated with and without the inclusion of interference terms.

**IV. THERMALIZATION IN AN ISOTROPIC HARMONIC TRAP**

We have shown in the previous section that the relation between the collision rate and the thermalization rate is strongly affected by partial wave interferences. In this section we emphasize the role played by the confinement, and we derive the dynamics of the thermalization in all collisional regime [21].

For the sake of simplicity, we consider the thermalization of an atomic mixture confined in a harmonic and isotropic trap:
\[
U_i(x, y, z) = \frac{1}{2} m_i \omega_i^2 (x^2 + y^2 + z^2).
\]

By application of the method of averages, we derive the following set of six coupled equations starting from the
evolution of the space-velocity correlations:

\[
\begin{align*}
\frac{d\langle r^2 \rangle_i}{dt} &= 2\langle r \cdot v_i \rangle_i, \\
\frac{d\langle r \cdot v_i \rangle_i}{dt} &= (\mathbf{v}_i^2 - \mathbf{v}_i^2) + \langle r \cdot v_i I_{ij} \rangle_i, \\
\frac{d\langle v_i^2 \rangle_i}{dt} &= -2\omega_i^2\langle r \cdot v_i \rangle_i + \langle v_i^2 I_{ij} \rangle_i.
\end{align*}
\]

(16)

The momentum and kinetic energy equations for the individual species include a contribution from the inter-species collision term, expressing the fact that it is the total momentum and total kinetic energy of the system rather than the individual species’ momentum and kinetic energy that are summational invariants. These dissipative contributions to the species equations do not appear in the equation for the radius since the collision is local and the number of atoms for each species is conserved.

In the absence of inter-species interactions the set of equations (16) describes the monopole mode of both species independently. The collision terms involving \( I_{ij} \) do not contribute to the above equations because all the dynamic quantities are collision invariant for intra-species collisions. This is why there is no damping for the breathing mode of a single-species classical gas confined in a harmonic isotropic trap. In this particular geometry and in the presence of two species, the relaxation only occurs through the inter-species collisions whatever the collisional regime of a given species may be.

The total number of inter-species collisions per unit of time \( \Gamma_{12} \) can be evaluated after the thermalization, once equilibrium has been reached:

\[
\Gamma_{12} = \frac{N_1 N_2 c(\sigma_{12})}{\pi^2 \sqrt{2}} \left( \frac{\mu \omega_1 \omega_2}{k_B T_f} \frac{(m_1 + m_2) \omega_1 \omega_2^2}{m_1 \omega_1^2 + m_2 \omega_2^2} \right)^{3/2}.
\]

(17)

As the initial state of the mixture is assumed to be not too far from the final state, this expression gives a reliable estimate of \( \Gamma_{12} \) during the thermalization process. The set of Eqs. (16) is exact within the Boltzmann formalism. To calculate quantitatively the relaxation driven by inter-species collisions, we make a Gaussian ansatz for the phase-space distribution function \( f_i \equiv f_i(\mathbf{r}, \mathbf{v}, t) \) of each species, with the inclusion of a factor taking into account the space-velocity correlations:

\[
f_i = N_i \exp \left( -\frac{m_i v_i^2 + m_i \omega_i^2 r^2}{2k_B T_i} \right) (1 + \eta_i m_i r v_i),
\]

(18)

where \( N_i \) is the normalization factor. The effective temperature \( T_i \) and the parameter \( \eta_i \) are the only time-dependent variables. Such an ansatz is inspired by the exact solution for the phase-space distribution function for the monopole mode, and provides a natural generalization of the local equilibrium distribution. For one species the Gaussian ansatz was shown to be accurate for investigating the damping of the coupled monopole-quadrupole oscillations in an anisotropic harmonic trap from the collisionless to the hydrodynamic regime.

At the lowest order, the space-velocity correlations only enter the momentum equations \( \langle r \cdot v_i I_{ij} \rangle \), while they can be neglected for the calculation of the term involving the kinetic energy \( \langle v_i^2 I_{ij} \rangle \). The details of this calculation can be found in Appendix B. We find:

\[
\langle r \cdot v_1 I_{12} \rangle = -\frac{m_1 \omega_1^2 (r \cdot v_1) - m_2 \omega_2^2 (r \cdot v_2)}{m_1 N_1 \omega_1 \omega_2},
\]

(19)

\[
\langle v_1^2 I_{12} \rangle = -\frac{m_1 (v_1^2) - m_2 (v_2^2)}{m_1 N_1 \tau},
\]

(20)

where the time constants \( \tau \) and \( \tau \) are given by:

\[
\begin{align*}
\frac{1}{\tau} &= \frac{4 \mu \omega_1 \omega_2}{3 m_1 \omega_1^2 + m_2 \omega_2^2} \langle \sigma_{12} \rangle \Gamma_{12}, \\
\frac{1}{\tau} &= \frac{8 \mu}{3 M} \langle \sigma_{12} \rangle \Gamma_{12}.
\end{align*}
\]

(21)

(22)

Combining Eq. (18) and Eqs. (19), (20), we obtain a closed set of six linear coupled equations. As a consequence, the relaxation in a trap does not correspond in general to a simple exponential decay.

We demonstrate the physics of rethermalization using a specific example in which \( m_1 = m_2 = m, \omega_1 = \omega_2 = \omega, N_1 = N_2 = N \) and keeping a constant cross section. However, we emphasize that the conclusions we draw are generic. In order to follow the thermalization it is convenient to introduce the three quantities:

\[
\begin{align*}
\Delta_1(t) &= \langle r^2 \rangle_1(t) - \langle r^2 \rangle_2(t), \\
\Delta_2(t) &= \langle r \cdot v_1 \rangle_1(t) - \langle r \cdot v_2 \rangle_2(t), \\
\Delta_3(t) &= \langle v_1^2 \rangle_1(t) - \langle v_2^2 \rangle_2(t).
\end{align*}
\]

We characterize the collisional regime through the quantity \( \omega_0 \) with \( \tau = N \tau \). The behavior we obtain is
reminiscent of the one of the monopole-quadrupole mode relaxation in a harmonic and anisotropic trap [17]. However, the observables $\langle r^2 \rangle_i$, $\langle r \cdot v_i \rangle_i$, and $\langle v^2 \rangle_i$ and their equation of evolution are not the same. The different regimes depend on the dimensionless parameter $\omega \tau_0$.

For $\omega \tau_0 \gg 1$, the gas is in the collisionless regime (see Fig. 2). We can recover formally the results obtained in the previous section, for a confinement of the gas in a box, by neglecting the space-velocity correlation term in the equation for $\Delta_3$, leading to an effective equation for thermalization that is identical to Eq. (11). In the harmonic confinement, $\Delta_3$ obeys a third order differential equation according to the set of equations (16).

In an anisotropic trap with different trap frequencies $\omega_{(x,y,z)}$, one can derive a set of equations similar to Eq. (16). In this case the behavior of the relaxation is also influenced by the damping of the quadrupole modes [17].

V. CONCLUSION

In this article, we have investigated the thermalization of a non degenerate atomic mixture. In our analysis we have taken into account both the energy and angular dependence of the inter-species elastic differential cross section. We have derived the explicit form for the thermalization rate, which depends on the interference between the partial waves while the collision rate does not. In addition, we have shown how the dynamics of the thermalization is modified by the collisional regime in presence of a confinement.

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The expansion of \( \Xi^1 \) leads to \( \Sigma^1 \). The expression for the coefficients \( \sigma_{1,2} \) for the distribution functions \( f_i \) allows for an expansion of \( \Xi^1 \) around the final temperature \( T_f \). We obtain

\[
\Sigma^{-} = \frac{\mu^2 V}{k_B T_f} \left( \frac{T_1 - T_2}{T_f} \right) N_1 N_2 \int d^3v_1 d^3v_2 d^2\Omega' \frac{d\sigma_{12}}{d\Omega'} [v_0 \cdot (v_r - v')] \Xi^1_{1,2}',
\]

(A1)

where we have introduced the quantity \( \Xi^1_{1,2}' = f_1(v'_1, t)f_2(v'_2, t) - f_1(v_1, t)f_2(v_2, t) \). The Gaussian ansatz for the distribution functions \( f_i \) allows for an expansion of \( \Xi^1_{1,2}' \) around the final temperature \( T_f \). We obtain

\[
\Sigma^{-} = -\frac{\mu^2 V}{k_B T_f} \left( \frac{T_1 - T_2}{T_f} \right) N_1 N_2 \int d^3v_1 d^3v_2 d^2\Omega' \frac{d\sigma_{12}}{d\Omega'} [v_0 \cdot (v_r - v')]^2 \exp \left( -\frac{M v_0^2 + v_r^2}{2k_B T_f} \right).
\]

(A2)

From the calculation of \( \Sigma^{-} \), one obtains the set of linear Eqs. 11 with the explicit form Eq. 12 for the relaxation times \( \tau \). The angular integration of Eq. A2 leads to the quantity \( \sigma_{12}(cx) \) defined in Eq. 13. From the expansion of the scattering amplitude in terms of partial waves 15, we can recast it in the form

\[
\sigma_{12}(cx) = \frac{2\pi}{k^2} \sum_{0 \leq l \leq l' < \infty} \alpha_{l,l'} \sin \delta_l \sin \delta_{l'} \cos(\delta_l - \delta_{l'}),
\]

(A3)

where we have introduced the dimensionless numerical factors \( \alpha_{l,l'} = (2 - \delta_{l,l'})((2l + 1)(2l' + 1) \int_0^1 (1 - x)P_l(x)P_{l'}(x), \delta_{l,l'} \) being the Kronecker delta symbol. The expression for the coefficients \( \alpha_{l,l'} \) explicitly contains terms describing interference between different partial waves. The properties of the coefficient \( \alpha_{l,l'} \) are the following: \( \alpha_{l,l'} > 0 \), \( \alpha_{l, l+1} < 0 \), \( \alpha_{l, l'} = 0 \) otherwise.

Finally, we perform the Gaussian integration of Eq. A2, and we work out the expression for the relaxation time \( \tau \) of Eq. 12 according to the notation of Eq. 11.

**APPENDIX B: COLLISION INTEGRALS CALCULATION FOR A HARMONIC CONFINEMENT**

The calculation of the quantity \( \langle v_r^2 I_{12} \rangle \) can be carried out in a way similar to the one used in Appendix A. The terms in \( \eta_i \) of the ansatz 13 do not contribute at the lowest order.

To calculate the quantity \( \langle r \cdot v_i I_{12} \rangle \), we introduce the quantities \( \Lambda_i = m_i N_i \langle r \cdot v_i I_{12} \rangle \) and \( \Lambda^\pm = \Lambda_1 \pm \Lambda_2 \). The global conservation of momentum ensures \( \Lambda^+ = 0 \). The first non-vanishing contribution to the linearized expansion of \( \Lambda^- \) is obtained by setting \( T_1 = T_2 = T_f \) in the ansatz 13. One finds:

\[
\Lambda^- = -\langle \eta_i - \eta_2 \rangle \mu^2 N_1 N_2 \int d^3v_0 e^{-\frac{M v_0^2}{2k_B T_f}}
\]

\[
\int d^3v_r d^2\Omega' \frac{d\sigma_{12}}{d\Omega'} [r \cdot (v_r - v')]^2 \exp \left( -\frac{M v_0^2 + v_r^2}{2k_B T_f} \right).
\]

(B1)

The ansatz 13 provides the explicit link between the space-velocity correlation moment and the parameters \( \eta_i = \langle r \cdot v_i I_{12} \rangle = 3\eta_i(k_B T_f)^2/(m_i \omega_i^2) \). This expression in combination with Eq. B1 permits one to derive the explicit expression 24 for the relaxation time \( \tilde{\tau} \) of the space-velocity correlation equation.
[19] The phase shifts for s, p, d, f and g partial waves as a function of the collision wave vector \( \vec{k} \) have been provided by S. Kokkelmans (Private Communication).