Appendix C

Thermal averaging

The total number of two-body collisions N between atoms of type a and b per unit trap volume V per unit time t is given by $n_a n_b \sigma(v_\mathrm{r}) v_\mathrm{r}$, where n_i is the density of i atoms, v_r the relative velocity of atom a with respect to atom b, and σ is the cross section. To get an average expression for the collision rate as a function of the atom cloud temperature T, we must consider the distribution $f(\vec{x}_a, \vec{x}_b, \vec{p}_a, \vec{p}_b)$ of atoms in a trap volume element dV with momenta (measured in the lab frame) $\vec{p}_a$ and $\vec{p}_b$. Further, we require the distribution function f to be unit normalized, i.e.

$$\int f(\vec{x}_a, \vec{x}_b, \vec{p}_a, \vec{p}_b) d^3x_a d^3x_b d^3p_a d^3p_b = 1 \ . \tag{C.1}$$

The thermally averaged value is then simply

$$\langle n_a n_b \sigma(v_\mathrm{r}) v_\mathrm{r} \rangle_T = \int n_a(\vec{x}_a) n_b(\vec{x}_b) \sigma(v_\mathrm{r}) v_\mathrm{r} f(\vec{x}_a, \vec{x}_b, \vec{p}_a, \vec{p}_b) d^3x_a d^3x_b d^3p_a d^3p_b \tag{C.2}$$

If the thermal de Broglie wavelengths of the atoms are small compared to the average spacing between atoms, then the gas can be treated with classical Maxwell-Boltzmann statistics. This condition can be stated numerically as

$$\left(\frac{1}{n}\right)^{1/3} \gg \frac{h}{\sqrt{3mk_BT}} \tag{C.3}$$

where m is the atomic mass, k_B is the Boltzmann constant, and T the cloud temperature. A 1 μK cloud of Rb atoms with density of the order 10^8 atoms/cm^3 easily falls into the classical regime. Assuming the cloud is in thermal equilibrium (or at least close to it) the canonical distribution function is given by the $f = C\exp(-H/k_BT)$, where H is the Hamiltonian of the system and C is a normalization constant. Moreover, in this classical regime we can neglect particle interactions. Accordingly, the

Hamiltonian for two particles in an isotropic harmonic trap is given by

$$H = \frac{1}{2m_a}\vec{p}_a{}^2 + \frac{1}{2m_b}\vec{p}_b{}^2 + \frac{1}{2}m_a\omega^2\vec{x}_a{}^2 + \frac{1}{2}m_b\omega^2\vec{x}_b{}^2 \tag{C.4}$$

where ω represents the trap frequency, and all coordinates and momenta are defined in the lab frame. (Trap anisotropies only effect the spatial density distribution of atoms, which is an experimentally measured quantity.) Next, H must be converted into the center-of-mass frame in the usual way by introducing center-of-mass and relative coordinates: where, $\vec{X}_{\rm cm} = m_a\vec{x}_a + m_b\vec{x}_b/(m_a + m_b)$, and $\vec{x}_{\rm r} = \vec{x}_a - \vec{x}_b$, $M = m_a + m_b$, $\mu = m_a m_b/(m_a + m_b)$. The transformed Hamiltonian is given by the expression:

$$H = \frac{1}{2M}\vec{P}^2_{\rm cm} + \frac{1}{2\mu}\vec{p}^2_{\rm r} + \frac{1}{2}M\omega^2\vec{X}^2_{\rm cm} + \frac{1}{2}\mu\omega^2\vec{x}^2_{\rm r}\ . \tag{C.5}$$

Equation C.2 can now be evaluated by inserting the center-of-mass Hamiltonian (Eq. C.5) into the distribution function, resulting in the following expression

$$\begin{aligned}\langle n_a n_b \sigma(v_{\rm r}) v_{\rm r}\rangle \quad &= \quad \frac{\int n_a(\vec{x}_a) n_b(\vec{x}_b)\, e^{-V(X_{\rm cm},x_{\rm r})/k_BT} d^3X_{\rm cm} d^3x_{\rm r}}{\int e^{-V(X_{\rm cm}+x_{\rm r})/k_BT} d^3X_{\rm cm} d^3x_{\rm r}} \times \\ &\qquad \frac{\int \sigma(v_{\rm r})\, v_{\rm r} e^{-T(p_{\rm r})/k_BT} d^3p_{\rm r}}{\int e^{-T(p_{\rm r})/k_BT} d^3p_{\rm r}}\ .\end{aligned} \tag{C.6}$$

Here, the Hamiltonian is written as sum of three terms, $H = T(P_{\rm cm}) + T(p_{\rm r}) + V(X_{\rm cm}, x_{\rm r})$. The center-of-mass momenta drops out of Eq. C.6 since the densities, cross section, and relative velocity have no explicit $\vec{P}_{\rm cm}$ dependence. Eq. C.6 can be separated into a term that depends only on the spatial coordinates and another term that depends only on the relative momenta. The spatially dependent term is effectively the total number of atoms N times the density-weighted-density $\langle DWD\rangle$,

$$N\langle DWD\rangle = \frac{\int n_a(\vec{x}_a) n_b(\vec{x}_b)\, e^{-V(X_{\rm cm},x_{\rm r})/k_BT} d^3X_{\rm cm} d^3x_{\rm r}}{\int e^{-V(X_{\rm cm},x_{\rm r})/k_BT} d^3X_{\rm cm} d^3x_{\rm r}} \tag{C.7}$$

which is an experimentally determined quantity. The remaining term is the thermal averaged rate constant K_2

$$\langle K_2\rangle = \frac{\int \sigma(v_{\rm r})\, v_{\rm r} e^{-T(p_{\rm r})/k_BT} d^3p_{\rm r}}{\int e^{-T(p_{\rm r})/k_BT} d^3p_{\rm r}}\ . \tag{C.8}$$

This expression can be simplified by evaluating the denominator and converting the integral over momenta to an integral over energy, $E = p_{\rm r}^2/2\mu$. The final expression for the thermal averaged rate constant is given by

$$\langle K_2 \rangle = 2\sqrt{\frac{2}{\mu\pi}}\,(k_B T)^{3/2} \int_0^\infty \sigma(E) E\, e^{-E/k_B T} dE \ . \tag{C.9}$$

Cold collision experimental observables are often the rate for some process to occur. Therefore, the standard definition for the thermal averaged cross section is taken to be

$$\langle \sigma \rangle = \frac{\langle K_2 \rangle}{\langle v_\mathrm{r} \rangle} = (k_B T)^{-2} \int_0^\infty \sigma(E) E\, e^{-E/k_B T} dE \ . \tag{C.10}$$

Finally, in cross-dimensional mixing experiments[108] such as the one used to observe the Feshbach resonance discussed in Section 5.2, the experimental observable is actually the rate of **energy** transfer[179]. In this case, the relevant thermal average is $\langle E K_2 \rangle$, i.e. the integral in equation C.9 must include an additional factor of E.