RAPID COMMUNICATION

Upper Limit for Quenching Rate Coefficient for cold electron–Metastable-Atom Collisions.

A S Dickinson
School of Natural Sciences, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK.
E-mail: A.S.Dickinson@ncl.ac.uk

Abstract. A simple model based on 100% quenching of metastables by threshold electrons transmitted to short distances on the polarization potential is employed. Values of the quenching rate coefficients of $1.6 \times 10^{-6}$ cm$^3$/s at threshold and $0.92 \times 10^{-6}$ cm$^3$/s at 50 K are estimated for electron collisions with metastable Xenon and $1.33 \times 10^{-6}$ cm$^3$/s at threshold for metastable Calcium.

PACS numbers: 34.80.Dp,37.10.Gh

28 September 2007

With the creation of ultracold neutral plasmas by photo-ionization of laser-cooled metastable atoms, the possibility arises of electron-atom interactions with temperatures as low as 100 mK (Killian et al., 2005; Killian, 2007). Electron collision energies at these temperatures are far below those traditionally studied by experiment or theory. Here we employ a simple model to estimate an upper bound for inelastic collision cross sections, primarily expected to be quenching, in collisions with neutral metastable atoms. Electron temperatures a few µs after photo-ionization have been measured (Roberts et al., 2004) to be around 50 K, relatively insensitive to the initial energy of the photo-electrons. Cold-collision electron-ion cross sections play an important role in three-body recombination, a critical process in the evolution of the plasma (Robicheaux and Hanson, 2003).

For an electron with energy equivalent to 100 mK the de Broglie wavelength is about 8000 $a_0$. Hence on approaching an atomic target the long-range attractive potential will lead to a large change in wavelength over a distance comparable to the wavelength. Such a change will give rise to quantum reflection of the electron. Only those electrons transmitted to short distances are assumed to give rise to quenching. Friedrich’s group (Moritz et al., 2001; Friedrich and Trost, 2004; Arnecke et al., 2006) have derived simple expressions for the probability, $P$, of near-threshold transmission to short distances on attractive long-range inverse-power potentials. Assuming 100% quenching when electrons reach short distances, the use of quantum reflection can yield a simple approximation to the quenching cross section. A similar model has been employed successfully for Penning ionization in collisions of cold metastable Helium.
Cold electron–Metastable-Atom Collisions

atoms (Dickinson, 2007). Note that for electron-ion collisions quantum reflection does not occur for motion on the Coulomb potential as the zero-energy limit is the semiclassical limit where typical actions are large compared to \( \hbar \) (Friedrich and Trost, 2004).

For a metastable rare-gas atom (apart from He) or a metastable alkaline-earth atom, the target will be in a P term so the leading long-range interaction is the charge quadrupole, varying as \( 1/R^3 \), \( R \) denoting the electron-atom separation. However this interaction is anisotropic and has zero expectation value for an \( s \)-state electron. The next term in the long-range interaction is due to the dipole polarizability of the target. Taking the spherical average of the polarizability, \( \bar{\alpha}_d \), since again the anisotropic component makes no contribution for \( s \)-states, the long-range potential can be approximated by

\[
V(R) = -\frac{\bar{\alpha}_d e^2}{2 \cdot 4\pi\epsilon_0 R^4}.
\]

For such a potential the transmission probability, \( \mathcal{P}_0 \), for \( s \)-waves close to threshold is (Moritz et al., 2001; Friedrich and Trost, 2004)

\[
\mathcal{P}_0(k) = 4k\beta, \quad \beta = \sqrt{\frac{m_e\bar{\alpha}_d e^2}{4\pi\epsilon_0\hbar^2}},
\]

where \( k \) denotes the electron’s wavenumber and \( m_e \) its mass. Assuming that all electrons reaching the inner region cause quenching, then the \( s \)-wave quenching cross section, \( \sigma_q^0(k) \), is given by

\[
\sigma_q^0(k) = \frac{\pi}{k^2} \mathcal{P}_0(k) = \frac{4\pi\beta}{k}.
\]

We note that \( \beta \) also happens to be the imaginary part of the scattering length for these collisions. Averaging \( \sigma_q^0(k) \) over a Maxwellian distribution at temperature \( T \), the \( s \)-wave contribution to the quenching rate coefficient, \( K_0^q(T) \), is given by

\[
K_0^q(T) = \frac{4\pi\hbar\beta}{m_e} \equiv 4\pi\sqrt{\frac{\bar{\alpha}_d e^2}{4\pi\epsilon_0 m_e}},
\]

independent of temperature. Since the unitarity limit is on the verge of being breached at the highest temperatures of interest we use, instead of equation (1), the modified \( s \)-wave tunnelling probability (Friedrich and Trost, 2004)

\[
\mathcal{P}_0(k) = 1 - \exp(-4k\beta),
\]

leading to the rate coefficient (Dickinson, 2007)

\[
K_0^q(T) = \frac{4\pi\hbar\beta}{m_e} \exp\left(\frac{T}{T_0}\right) \text{erfc}\left(\sqrt{\frac{T}{T_0}}\right), \quad T_0 = \frac{\hbar^2}{8m_e k_B \beta^2}.
\]

Arnecke et al. (2006) have obtained additional terms in the power-series expansion for \( \mathcal{P}_0(k) \) to that employed in equation (1). Using \( \mathcal{P}_0 \) from these terms instead of from equation (3) gives a difference in the value of \( \mathcal{P}_0 \) of less than 5%.
Calculating similarly the $p$-wave contribution to the quenching cross section, $\sigma_1^q(k)$, yields, using the near-threshold result for tunnelling through the centrifugal barrier, (Moritz et al., 2001; Friedrich and Trost, 2004)

$$\sigma_1^q(k) = 4\pi k \beta^3 / 3,$$

and the corresponding contribution to the quenching rate coefficient, $K_1^q(T)$, is,

$$K_1^q(T) = \frac{4\pi \hbar \beta}{m_e} \frac{T}{8T_0}. \quad (5)$$

We discuss below the importance for $p$-waves of the anisotropic potential.

The analogous calculation for the $d$-wave contribution yields

$$K_2^q(T) = \frac{4\pi \hbar \beta}{m_e} \frac{1}{27} \left( \frac{T}{8T_0} \right)^2$$

and the $d$-wave contribution is negligible at temperatures for which the approximations leading to the $s$-wave result, equation (4), are valid.

For metastable Xe, where an ultracold plasma has been created by Killian et al. (1999), the dipole polarizability tensor has been measured (Molof et al., 1974), $\bar{\alpha}_d = 429 \text{ a}_0^3$, yielding $\beta = 20.7 \text{ a}_0$ and the low-temperature limit $K_0^q(T) = 1.6 \times 10^{-6} \text{ cm}^3/\text{s}$. Results from equation (4) for higher temperatures, including the $p$-wave contribution from equation (5), are shown in figure 1, along with the $p$-wave contribution itself. For metastable Xe the value of $T_0$ (see equation (4)) is 92 K and this temperature gives an estimate of the upper limit for the validity of this model.

Given a metastable Xe density of $10^{11} \text{ cm}^{-3}$ (Killian et al., 2005) this value of the threshold rate coefficient would give an initial loss rate of ultra-cold electrons of $1.6 \times 10^5 \text{ /s}$. Although this loss rate is slow compared to the initial loss rate of electrons due to expansion (Simien et al., 2004), most of the photo-electrons remain in the centre of the initial cloud.

For the $p$-wave interaction we must take account of the leading anisotropic part, $V_{an}(R)$, of the electron-atom interaction:

$$V_{an}(R) = -\frac{1}{4\pi \epsilon_0} \left( \frac{e Q}{R^3} + \frac{e^2 \alpha_2}{2R^4} \right) P_2(\cos \theta), \quad (6)$$

where $Q$ is the quadrupole moment, $\alpha_2$ the anisotropic dipole polarizability, $P_2(x)$ the second Legendre polynomial and $\theta$ is the angle between the target quantization axis and the electron-atom line. For metastable Xe the value of $Q = 0.30 \text{ a}_u$ has been measured by Sandars and Stewart (1972) and the value of $\alpha_2 = -41.1 \text{ a}_u^3$ has been measured by Molof et al. (1974).

While quantal reflection on the combination of an $R^{-3}$ and an $R^{-4}$ potential has been considered (Friedrich and Trost, 2004), this was in the context of atom-surface scattering and hence only the $s$-wave solution was of interest. Even ignoring the reduction in the effective $C_3$ coefficient arising from the angular integration, the
transmission probability from the quadrupole potential would be \( P_p = 0.1(ka_0)^3 \), to be compared to \( 9.2(ka_0)^3 \) from the mean polarizability. Hence, to the accuracy of the approximations being employed here, the quadrupole contribution can be ignored. Similarly, again neglecting the angular integration factors for the anisotropic polarizability, its contribution is about 10% that of the mean polarizability so the anisotropic polarizability contribution can also be ignored. Since the quadrupole moments of metastable Ne, Ar, and Kr are about 15% that of metastable Xe (Sandars and Stewart, 1972) and the anisotropic polarizabilities are a smaller fraction of the mean polarizability for these gases than for Xe, (Molof et al., 1974), use of the mean polarizability only for the other metastable rare gases should again be valid.

For metastable Ne, which has been trapped at a temperature of about 1 mK (Kuppens et al., 2002), the quenching rate coefficient upper bound is \( 1.06 \times 10^{-6} \text{ cm}^3/\text{s} \).
in the low-temperature limit, using the value of the mean polarizability measured by Molof et al. (1974).

For metastable Ca, which has been trapped at a temperature of 0.13 mK (Hansen et al., 2003), the quenching rate coefficient upper bound is $1.33 \times 10^{-6}$ cm$^3$/s in the low-temperature limit, using the value of the mean dipole polarizability calculated by Mitroy and Bromley (2004). In this case the value of $T_0$ is 133 K. Values of the quenching rate coefficient are shown in Figure 1. The value of the quadrupole moment, 12.96 a.u., (Mitroy and Bromley, 2004) is much larger than those of the metastable rare gases. The value of the polarizability anisotropy is $-28.36 a_0^3$ (Mitroy and Bromley, 2004) so that at the distances of interest the quadrupole term in equation (6) is dominant.

However, for an anisotropy of the form $v_2(R)P_2(\cos \theta)$, the diagonal matrix elements for a $p$-wave electron (spin ignored) colliding with a $3P_2$ target are $7v_2/50, -7v_2/50$ and $v_2/50$ for total angular momentum, atom and relative motion, $J = 1, 2$ and 3, respectively, using the matrix elements from Reid (1973). In the most favourable case, $J = 1$, the transmission probability for the quadrupole potential is $0.63(ka_0)^3$, compared to $7.6(ka_0)^3$ for the spherical polarizability value. Hence, to the accuracy of this approximation, the anisotropic contribution can be ignored. For the other alkaline earths broadly similar long-range anisotropic potentials occur relative to the isotropic polarization interaction (Mitroy and Bromley, 2004), so the estimate from equation (5) of the $p$-wave contribution should be adequate.

While an ultracold plasma has also been created in Sr (Simien et al., 2004), this was produced from trapped ground-state atoms.

This upper-bound estimate obtained using equations (4) and (5) should be useful in further simulation of the evolution of these ultracold plasmas (Robicheaux and Hanson, 2003).

Acknowledgments

We thank Professor Robicheaux for valuable comments.

References