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LETTER TO THE EDITOR

Analytical expressions for cross sections of Rydberg–neutral inelastic collisions

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Abstract. We obtain simple analytical expressions for the cross sections of the state-changing and ionisation collisions of Rydberg atoms with neutral atomic particles due to the Rydberg-electron–perturber interaction. The theoretical investigation is based on the impulse approximation and binary encounter approach for the form factor. The earlier results of Alekseev and Sobel'man and Omont turn out to be the limiting cases of our expressions. The calculated quenching cross sections for the Rydberg states agree well with experimental results and numerical calculations.

Considerable attention is devoted at present to collisions involving Rydberg atoms and various theoretical investigations of state-changing collisions between Rydberg atoms and neutral atomic or molecular targets have been made (see Hickman *et al* 1983, Matsuzawa 1983 and references therein). In most papers the theoretical cross sections for transitions between the Rydberg states due to the electron–perturber interaction were obtained only after very time consuming numerical calculations. Exceptions are the broadening and shift cross sections of Alekseev and Sobel'man (1965), the expressions of Omont (1977) for summed and broadening cross sections, an approximate scaling formula of Hickman (1981), an adiabatic approximation of Kaulakys (1982), and elastic broadening and shift cross sections of Kaulakys (1984).

Here we present theoretical expressions for the cross sections of state-changing collisions between the Rydberg atom and a structureless neutral atomic particle. Our investigation is based on the impulse approximation and the binary encounter approach for the form factor. We shall calculate the cross section for a $nl \to n'$ transition, where n' is a hydrogenic manifold. This cross section is given by the following relation

$$\sigma_{nl,n'} = \frac{2\pi}{v^2} \int_{|\Delta E|/v}^{\infty} |f_e(Q)|^2 F_{nl,n'}(Q) Q \, dQ \qquad (1)$$

where v is the relative velocity of the colliding partners, $f_e(Q)$ is the electron–perturber scattering amplitude for a given momentum transfer Q, $F_{nl,n'}(Q)$ is the squared form factor, and $\Delta E = (2n^{*2})^{-1} - (2n'^2)^{-1}$ is the energy defect involved in the transition with n^* the effective principal quantum number of the initial state. We can use the form factor given by the binary encounter theory (see Matsuzawa 1974)

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$$F_{nl,n'}(Q) = \frac{1}{2n'^3 Q} \int_{\rho_0}^{\infty} |g_{nl}(\rho)|^2 \rho \, d\rho \qquad \rho_0 = |\Delta E - \tfrac{1}{2}Q^2|/Q \qquad (2)$$

where $g_{nl}(\rho)$ is the radial wavefunction of the Rydberg electron in the momentum space. The validity of this approximation in Rydberg-neutral collisions has been recently investigated by Gounand and Petitjean (1984). It is important to note that in the calculation of the cross section according to equations (1) and (2), ΔE in the expression for ρ_0 may be neglected. That is why $|\Delta E| \ll \frac{1}{2}Q_{\min}^2 = (\Delta E)^2/2v^2$ if $|\Delta E| \gg 2v^2$ and the contribution to the integral (1) of the integration over Q in the interval $|\Delta E|v^{-1} \leqslant Q \leqslant (2\Delta E)^{1/2}$ (when $\frac{1}{2}Q^2 \leqslant |\Delta E|$) is small if $|\Delta E| \leqslant 2v^2$ and $v^2 n'^3 \leqslant 1$. Thus substitution of equation (2) in equation (1) and integration by parts yields

$$\sigma_{nl,n'} = \frac{2\pi L^2}{v^2 n'^3} \int_{\rho_t}^{\infty} |g_{nl}(\rho)|^2 (\rho - \rho_t)\rho \, d\rho \tag{3}$$

where $\rho_t = |\Delta E|/2v$ and the scattering amplitude $f_e(Q)$ has been replaced by the scattering length L.

In the case $n' = n$ we recover the result of Omont (1977), $\sigma_{nl,n} = 2\pi L^2/(v^2 n^3)$.

Using the distribution (see Omont 1977)

11057 $$|g_{n0}(\rho)|^2 = 4\pi^{-1} n^* \rho^{-2} (1 + n^{*2}\rho^2)^{-2} \qquad (2n^{*2})^{-1} \leqslant \rho \leqslant 1$$

for states such that $l \ll n$, and

$$|g_n(\rho)|^2 \equiv \frac{1}{n^2} \sum_{l=0}^{n-1} (2l+1)|g_{nl}(\rho)|^2 = 32\pi^{-1} n^3 (1 + n^2\rho^2)^{-4}$$

for the whole set of sublevels of n, we easily derive expressions for the cross sections

$$\sigma_{n(l),n'} = \frac{2\pi L^2}{v^2 n'^3} \mathscr{I}_{n(l)}(\xi) \qquad \xi = \frac{|\Delta E| n^*}{2v} \tag{4}$$

$$\mathscr{I}_{n0}(\xi) = 2\pi^{-1}[\cot^{-1}\xi - \xi \ln(1 + \xi^{-2})] \qquad \xi \leqslant n \tag{5}$$

$$\mathscr{I}_n(\xi) = 2\pi^{-1}[\cot^{-1}\xi - \tfrac{1}{3}\xi(5 + 3\xi^2)(1 + \xi^2)^{-2}]. \tag{6}$$

The limiting forms of the functions $\mathscr{I}_{n0}(\xi)$ and $\mathscr{I}_n(\xi)$ are

$$\mathscr{I}_{n0} = 1 - 2\pi^{-1}\xi(2\ln\xi^{-1} + 1) + \ldots \qquad \mathscr{I}_n = 1 - \tfrac{16}{3}\pi^{-1}\xi + \ldots \qquad \xi \ll 1 \;\; (\xi \leqslant 0.2)$$

$$\mathscr{I}_{n0} = \tfrac{1}{3}(\pi\xi^3)^{-1}(1 - \tfrac{4}{5}\xi^{-2} + \ldots) \qquad \mathscr{I}_n = \tfrac{16}{15}(\pi\xi^5)^{-1}(1 - \tfrac{15}{7}\xi^{-2} + \ldots) \qquad \xi \gg 1 \;\; (\xi \geqslant 3).$$

From equations (4)–(6) we may calculate cross sections summed over n', $\sigma_{nl} = \Sigma_{n'} \sigma_{nl,n'}$. When $n^2 \gg v^{-1}$ the discrete sum may be replaced by an integral. Therefore, integration of equation (3) by parts yields

$$\sigma_{nl} = \frac{2\pi L^2}{v^2} \int_{-\infty}^{+\infty} d(\Delta E) \int_{\rho_t}^{\infty} |g_{nl}(\rho)|^2 (\rho - \rho_t)\rho \, d\rho = \frac{4\pi L^2}{v} \int_0^{\infty} |g_{nl}(\rho)|^2 \rho^3 \, d\rho \tag{7}$$

which is identical with the results of Alekseev and Sobel'man (1965) and Omont (1977).

By analogy we may estimate the ionisation cross section

$$\sigma_{nl}^{i} = \frac{2\pi L^2}{v^2} \int_{|E_i|}^{\infty} d(\Delta E) \int_{\rho_t}^{\infty} |g_{nl}(\rho)|^2 (\rho - \rho_t)\rho \, d\rho$$

$$= \frac{2\pi L^2}{v} \int_{\rho_i}^{\infty} |g_{nl}(\rho)|^2 (\rho - \rho_i)^2 \rho \, d\rho \tag{8}$$

where $\rho_i = |E_i|/2v = (4vn^{*2})^{-1}$. Finally we have

$$\sigma^{i}_{n(l)} = 2\pi L^2 v^{-1} \mathscr{I}^{i}_{n(l)}(\xi_i) \qquad \xi_i = n^*\rho_i = (4vn^*)^{-1} \tag{9}$$

$$\mathscr{I}^{i}_{n0}(\xi_i) = 2(\pi n^*)^{-1}[1 + \xi_i^2 \ln(1+\xi_i^{-2}) - 2\xi_i \cot^{-1}\xi_i] \qquad \xi_i \leqslant n \tag{10}$$

$$\mathscr{I}^{i}_{n}(\xi_i) = 4(\pi n)^{-1}[(\xi_i^2 + \tfrac{2}{3})(\xi_i^2+1)^{-1} - \xi_i \cot^{-1}\xi_i]. \tag{11}$$

The limiting forms of the functions $\mathscr{I}^{i}_{n0}(\xi_i)$ and $\mathscr{I}^{i}_{n}(\xi_i)$ are

$$\mathscr{I}^{i}_{n0} = 2(\pi n^*)^{-1}(1 - \pi\xi_i + \ldots)$$

$$\mathscr{I}^{i}_{n} = \tfrac{8}{3}(\pi n)^{-1}(1 - \tfrac{3}{4}\pi\xi_i + \ldots) \qquad \xi_i \ll 1$$

$$\mathscr{I}^{i}_{n0} = \tfrac{1}{3}(\pi n^* \xi_i^2)^{-1}(1 - \tfrac{2}{5}\xi_i^{-2} + \ldots)$$

$$\mathscr{I}^{i}_{n} = \tfrac{8}{15}(\pi n \xi_i^4)^{-1}(1 - \tfrac{10}{7}\xi_i^{-2} + \ldots) \qquad \xi_i \gg 1.$$

The expressions obtained for the Rydberg-neutral inelastic scattering cross sections may be used for a wide variety of systems. The loss of information on $nl \to n'l'$ processes is not very important since most measurements only provide the total depopulation cross sections. On the other hand, as there is no selection rule for l', the cross section for the $nl \to n'l'$ transition with $l \sim 1$ is of the order $\sigma_{nl,n'}/n'$. When the final n' state is not entirely hydrogenic, the cross section for the transition to the degenerate hydrogenic

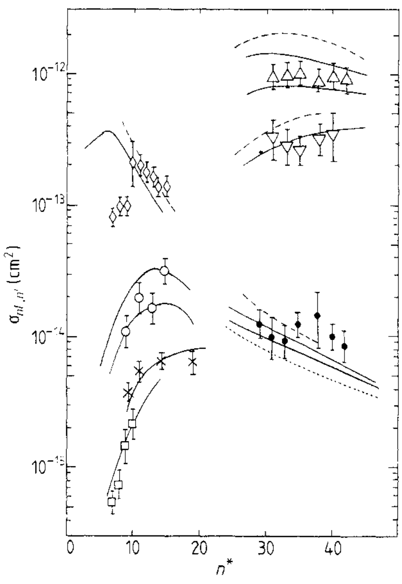

Figure 1. Semi-logarithmic plots of the cross sections for the quenching of the Na and Rb Rydberg states by He and Xe as a function of n^*. Experiment: ◊, Na(nd)+He, $T = 430$ K, Gallagher *et al* (1977); ○, Rb(ns)+He, $T = 520$ K, Hugon *et al* (1980); ×, Rb(np)+He, $T = 460$ K, Gounand *et al* (1977); □, Na(ns)+He, $T = 425$ K, Gallagher and Cooke (1979); △, Rb(ns)+Xe, $T = 296$ K, Hugon *et al* (1982); ▽, Rb(nd)+Xe, $T = 296$ K, Hugon *et al* (1982); ●, Rb(ns)+He, $T = 296$ K, Hugon *et al* (1982). Theory: full curves, equation (4) multiplied by $(n' - l_0)/n'$ with $L_{He} = 1.14$, $L_{Xe} = -5.8$; $\delta_s = 1.35$, $\delta_d = 0.014$ for Na, $\delta_s = 3.14$ and 3.20 if $5 \leqslant n^* \leqslant 20$, $\delta_s = 3.16$ and 3.24 if $25 \leqslant n^* \leqslant 45$, $\delta_p = 2.65$, $\delta_d = 1.40$ for Rb; broken curves, Born approximation with a Fermi pseudopotential (Hugon *et al* 1982) for large n^* values and impulse approach (Gounand and Petitjean 1984) for low n^* values; dotted curve, scaling formula of Hickman (1981).

manifold with $l' \geqslant l_0$ (where l_0 is the smallest orbital momentum of the degenerate states) may be expressed as $\sigma^{(l_0)}_{nl,n'} \simeq \sigma_{nl,n'}(n'-l_0)/n'$. When the scattering length approximation for the scattering of the electron by a neutral atomic particle is not appropriate, in equations (3)-(4) and (7)-(9) L^2 should be replaced by $\bar{\sigma}_e/4\pi$, where $\bar{\sigma}_e$ is the electron-perturber elastic scattering cross section averaged over the quantum distribution of the electron velocities in the Rydberg nl state.

In figure 1 examples of the comparison of the present theoretical quenching cross sections with experimental results and other calculations are shown. It should be noted that the cross sections are very sensitive to the energy defect involved in the transition if $\xi \geqslant 0.1$. The energy differences between the isolated nl state and the nearest hydrogenic manifolds equals $\{\delta_l\}/n^{*3}$, and $(\{\delta_l\}-1)/n^{*3}$, where $\{\delta_l\}$ is the fractional part of the quantum defect. For Rb(ns) states the quantum defect is not a constant but fluctuates between 3.14 and 3.24 when $10 \leqslant n \leqslant 50$ (see Moore 1952, Liberman and Pinard 1979). That is why the Rb(ns) state quenching cross sections are calculated for two quantum defects. The theory is in reasonable agreement with experiments and results of numerical calculations at $n^* \geqslant 10$ especially taking into account that the present calculations are performed without averaging over the collision velocity. We do not know of any experimental measurements of the collisional ionisation cross sections of the very highly excited Rydberg atoms by structureless neutral atomic particles and therefore we cannot present a comparison between the theoretical and experimental ionisation cross sections.

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