Resonances in electron capture total cross sections for ion-H(1s) collisions

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Abstract. We have calculated charge transfer total cross sections in ion-H(1s) collisions at very low energies ($E < 1$ eV). These cross sections show a Langevin-type behaviour, although the corresponding transition probabilities are smaller than one, as obtained in the Landau-Zener model. The cross sections exhibit numerous spikes which are related to the existence of resonant states in the adiabatic potential of the quasi-molecule formed during the collision.

1. Introduction

Charge transfer (CT) reactions are important processes in astrophysical and fusion plasmas. In particular, reactions between low-charged ions and H are relevant in HII regions and planetary nebulae (see e.g. [1]), while CT involving highly charged ions and H are important processes in fusion plasmas. In previous works [2, 3, 4, 5], we have employed close-coupling expansions in terms of molecular wave functions to study the CT reactions from low to intermediate energies. In this work we address the very low energy regime (0.001 eV$< E <$1 eV), where resonances in the CT cross section show up. In this study, we use the potential energy curves and non-adiabatic couplings obtained in previous works, and a quantal treatment for the dynamics that includes a common reaction coordinate (see [6] and references therein) to ensure that the expansion fulfills the collision boundary conditions. In the present work we report total cross sections for CT in collisions with H(1s) of O^{2+}, N^{2+}, C^{4+} and B^{5+} with H(1s).

2. Theory

For each value of the total angular momentum, J, the collisional wave function, Ψ^J, is expanded in terms of the molecular functions ϕ_k in the form:

$$\Psi^J(\boldsymbol{r}, \boldsymbol{\xi}) = \sum_k \chi_k^J(\boldsymbol{\xi}) \phi_k(\boldsymbol{r}, \xi) \tag{1}$$

where the functions ϕ_k are (approximate) eigenfunctions of the clamped-nuclei electronic Hamiltonian in the Born-Oppenheimer approximation, and $\boldsymbol{\xi}$ is the common reaction coordinate. Substitution of the expansion (1) in the stationary Schrödinger equation leads to a set of differential equations, whose solutions are the nuclear functions χ_k^J. The scattering matrix

$\boldsymbol{S}^J$ is then calculated from these nuclear functions, and the total cross section for transition from the state i to the state j is given by:

$$\sigma_{ij}(E) = \frac{\pi}{k_i^2} \sum_J (2J+1)|S_{ij}^J|^2 \tag{2}$$

At low energies, the CT cross section is usually estimated using the classical Langevin formula (see e.g. [7]):

$$\sigma_{\rm L}(E) = \pi b_{max}^2 = \pi q (2\alpha/E)^{1/2} \tag{3}$$

The Langevin model assumes that the CT process takes place with probability equal to one for impact parameters smaller than b_{max}, which is the impact parameter that leads to orbiting, and the interaction potential is approximated by $V(R) = -0.5q^2\alpha/R^4$, with q the charge of the ion and α the atom polarizability. For the systems considered in this work, a more realistic approximation is obtained by employing the Landau-Zener (see e.g. [8]) transition probability. This leads to what we call the Landau-Zener-Langevin (LZL) model:

$$\sigma \simeq 4\pi \int_0^{b_{\rm max}} bp(1-p){\rm d}b \tag{4}$$

where

$$p = \exp\left(\frac{-2\pi H_{12}^2}{a v_r}\right),\ a = \frac{{\rm d}(H_{22}-H_{11})}{{\rm d}R} \ \text{ and } \ v_r = v\left(1 - \frac{H_{11}(R_0)}{E} - \frac{b^2}{R_0^2}\right)^{1/2} \tag{5}$$

3. Results

In $O^{2+}(2s^2 2p^2\ ^3P)$+H(1s), the entrance channel correlates to molecular states $^{2,4}\Sigma^-$ and $^{2,4}\Pi$. The total CT cross section is then expressed as:

$$\sigma = \frac{2}{9}\left[\sigma(^4\Sigma^-) + \sigma(^4\Pi_-) + \sigma(^4\Pi_+)\right] + \frac{1}{9}\left[\sigma(^2\Sigma^-) + \sigma(^2\Pi_-) + \sigma(^2\Pi_+)\right] \tag{6}$$

where $\sigma(i)$ is the CT cross section for the collision with the molecular entrance channel of a given symmetry and multiplicity, and the subindexes + and − indicate the symmetry of the Π wave functions under reflection in the collision plane. At low energies, the CT process takes place through transitions to the molecular states $^4\Sigma^-$ and $^4\Pi$ dissociating into $O^+(2s2p^4\ ^4P)$+H^+ (see figure 1), in the avoided crossings at $R \simeq 4$ a$_0$ between the $^4\Sigma^-$ energy curves, and $R \simeq 4.5$ a$_0$ between the $^4\Pi$ ones. So that, the minimal basis set for evaluating the CT cross section includes six molecular states: two states $^4\Pi_+$, symmetric under reflection in the collision plane, and four antisymmetric states $^4\Sigma^-$, $^4\Pi_-$.

In figure 3 we plot the cross sections $\sigma(^4\Pi_+)$ and $\sigma(^4\Sigma^-) + \sigma(^4\Pi_-)$, which exhibit many spikes. For $\sigma(^4\Pi_+)$, we have assigned these spikes to shape resonances in the adiabatic entrance channel by analyzing the contribution to the cross section of each partial wave and with the help of the program Level 7.7 [9]. The numbers (v, J) indicate the vibro-rotational quantum numbers of the quasi-bound states. For some resonances, a single index J has been employed, since the energy of the corresponding state lies above the maximum of the effective potential. With respect to the calculation in the antisymmetric subsystem, we have found that the resonant structures of the contributions $\sigma(^4\Sigma^-), \sigma(^4\Pi_-)$ cannot be assigned to quasi-bound states of any of the initial molecular states because of the superposition of these two states induced by the rotational coupling. On the other hand, the calculated cross sections are significantly smaller than predicted by the Langevin model; however, the LZL formula of Eq. (4) yields a reasonable agreement with the calculated values.

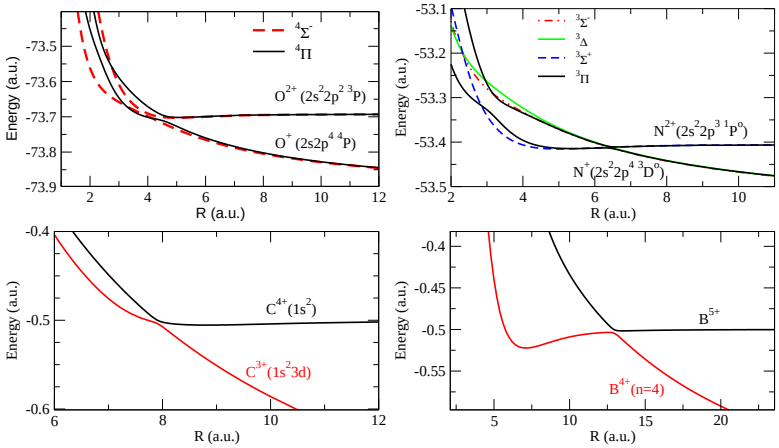

Figure 1. Relevant potential energy curves for the charge transfer process at low energy between the ion (indicated in the figure) and H(1s). The asymptotic state of the projectile is indicated in each graph.

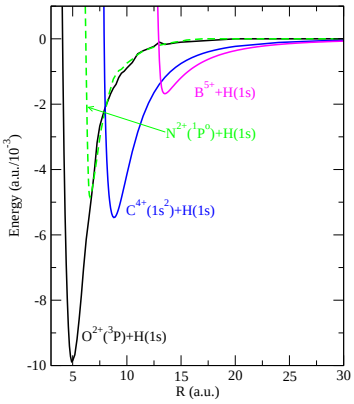

Figure 2. Adiabatic entrance potential energy curves for the four systems illustrated in this work.

The total CT cross section in $N^{2+}(2s^22p^2P^o)$+H(1s) collisions is given by the expression:

$$\sigma = \frac{1}{12}\left[\sigma(^1\Sigma^+) + \sigma(^1\Pi_-) + \sigma(^1\Pi_+)\right] + \frac{3}{12}\left[\sigma(^3\Sigma^+) + \sigma(^3\Pi_-) + \sigma(^3\Pi_+)\right] \qquad (7)$$

At low energies, the main mechanism involves transitions in the neighbourhood of the avoided crossing at $R \simeq 6.4$ a$_0$ between the entrance channels of symmetry $^3\Pi$ and those of the same symmetry and multiplicity correlating to $N^+(2s^22p^4\,^3D^o)$+H^+ (see Fig. 1). As for the case of O^{2+}+H collisions, the cross section $\sigma(^3\Pi_-)$ shows many resonances that can be assigned to quasi-bound levels of the entrance channel potential, while the shape of the cross section $\sigma(^3\Sigma^+) + \sigma(^3\Pi_+)$ is strongly modified by the rotational couplings. The LZL model yields reasonable agreement with the calculated values; however, for $E > 0.1$ eV there are important contributions to the calculated cross section of transitions in a second avoided crossing at $R \simeq 3$ a$_0$, not considered in the LZL model.

In the case of C^{4+}+H(1s) collisions, the active electron interacts with the H^+ nucleus and with the $C^{4+}(1s^2)$ core, and the latter interaction has been described by means of a model potential. The CT reaction takes place through transitions from the entrance channel $C^{4+}(1s^2)$+H(1s) to the molecular orbitals dissociating into $C^{3+}(1s^2n{=}3)$+H^+. In particular, at low energies, the entrance channel is depopulated via transitions to the molecular orbital dissociating into $C^{3+}(1s^23d)$+H^+ (see Fig. 1); this is illustrated in Fig. 3, where we compare a 2-state calculation with those from the 20-state basis set of [5]. The CT cross section of Fig. 3 shows many resonant structures, including below- and above-the-barrier resonances.

In B^{5+}+H(1s) collisions, the main mechanism of the CT process involves 5gσ-4fσ transitions in the corresponding avoided crossing at $R \simeq 12.9$ a$_0$ (see Fig. 1). In the calculation we have employed a 12-term molecular basis set that includes entrance channel, the molecular orbitals dissociating into $B^{4+}(n=4)$+H^+ and the orbital 6hσ, which correlates to $B^{4+}(n=5)$+H^+. At $R < 12.9$ a$_0$, the adiabatic potential energy curve of the entrance channel increases as $4/R$, and therefore, this potential shows a shallow minimum that supports a relatively small number of quasi-bound states (see Fig. 2).

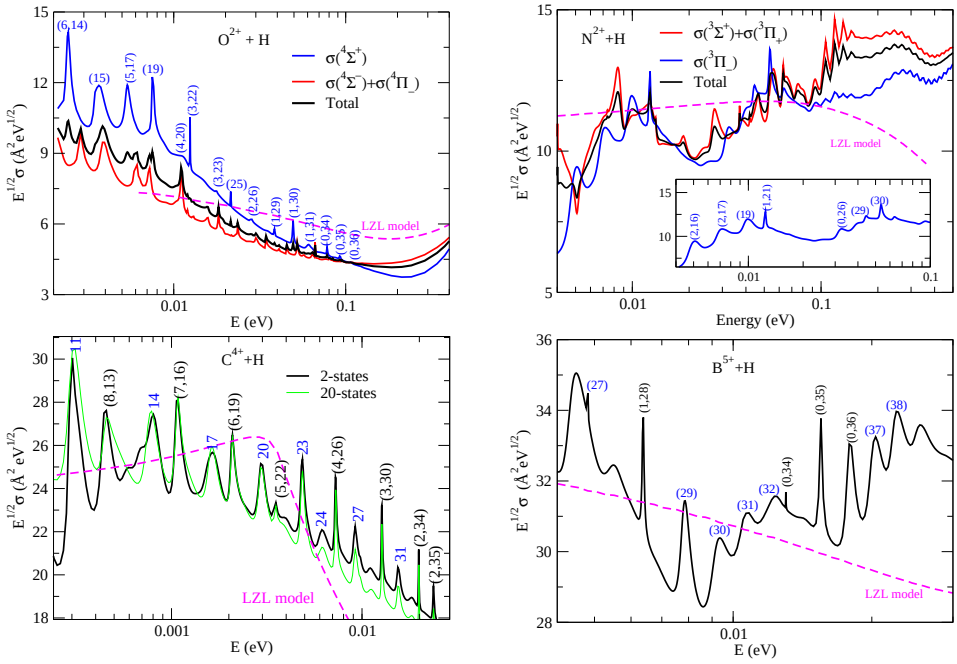

Figure 3. Scaled charge transfer cross sections. The labels on the spikes correspond to the quantum numbers (ν, J) or only J. In each graph, the dashed line has been obtained by applying the model of Eq. (4) to the relevant avoided crossing illustrated in figure 1.

4. Conclusions

We have calculated charge transfer cross sections for several systems using a quantal molecular treatment. In all cases, we have found the presence of spikes which correspond to shape resonances in the entrance channel adiabatic potential. Some spikes are produced by particular quasi-bound states of the effective potential, and have been assigned the corresponding pair of quantum numbers (ν, J), while others correspond to states above the barrier, and only (J) has been given. We have also shown that the CT cross sections oscillate around the estimate of the semiclassical Landau-Zener-Langevin model.

Acknowledgments

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References

[1] D. Pequignot. *Astron. Astrophys.*, 81:356, 1980.

[2] C. N. Cabello, L. F. Errea, L. Fernández, L. Méndez, A. Macías, I. Rabadán, and A. Riera. *J. Phys. B: At. Mol. Opt. Phys.* **36** 307 (2003)

[3] P. Barragán, L. F. Errea, L. Méndez, A. Macías, I. Rabadán, and A. Riera. *Phys. Rev. A* **70** 022707 (2004)

[4] L. F. Errea, F. Guzmán, C. Illescas, L. Méndez, B. Pons, A. Riera, and J. Suárez. *Plasma Phys. Control. Fusion* (Submitted) (2006)

[5] L. F. Errea, J. D. Gorfinkiel, C. Harel, H. Jouin, A. Macías, L. Méndez, B. Pons, and A. Riera. *J. Phys. B: At. Mol. Opt. Phys.* **32** L673 (1999)

[6] L. F. Errea, C. Harel, H. Jouin, L. Méndez, B. Pons, and A. Riera. *J. Phys. B: At. Mol. Opt. Phys.* **31** 3527 (1998)

[7] C. N. Liu, A. T. Le, and C. D. Lin. *Phys. Rev. A* **68** 062702 (2003)

[8] B. H. Bransden and M. H C. McDowell. *Charge Exchange and the Theory of Ion-Atom Collisions.* Oxford, Clarendon, (1992)

[9] R.J. Leroy. Level7.7: A computer program for solving the radial Schrödinger equation for bound and quasibound levels. University of Waterloo, Chemical Physics Research Report CP-661 (2005)