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Theoretical investigation of the electron capture in collisions of O^{8+} ion with H and He atoms: Comparison between the Landau–Zener and the over-barrier models

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Abstract

Analytical and semi-analytical theories based on the molecular and classical treatments have been applied for electron capture processes in collisions of hydrogen and helium atoms with low energy ($E = 0.1, \ldots, 10$ keV/amu) O^{8+} bare ion impact. The used Landau–Zener model (LZ), which allows to give analytical formulas for the cross-sections in our recent approach and the modified over-barrier model (OBM) [Phys. Rev. A 62 (2000) 042711] are briefly summarized. The obtained values of the LZ and OBM cross-sections are compared with experimental data and the results of other sophisticated numerical calculations. It is found that the LZ model provides much reliable cross-sections for charge transfer than the OBM model.

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1. Introduction

Electron capture into slow ($v < 1$ a.u.) highly charged ions (HCIs) interacting with neutral gas atoms is quite an important collision process in the atomic physics, plasma physics and astrophysics. State selective and total charge exchange cross-section data are essential for modeling and diagnostics of astrophysical plasmas or laboratory fusion plasmas. The electron capture in collisions of HCIs with H and He atoms plays central role in particular case of the radiative plasma cooling in edge plasmas and the periphery of Tokamak fusion plasma. In a laboratory plasma, the impurity ions interact with neutral beams of H and He injected into the plasma and the mechanism of single electron capture (SEC) as well as double electron capture (DEC) can experimentally be studied by radiative, energy gain and Auger electron spectroscopy.

The present theoretical work dealing with the electron capture in collision of HCI with H and He atom was motivated by a recently published modified over-barrier model (OBM) worked out for the process [1]. It was interesting to compare the performance of this approach with that of the widely used Landau–Zener (LZ) theory, because

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the LZ and the OBM theories today are well developed and have rather different physical content.

In this paper we present calculations of SEC and DEC cross-sections in the projectile energy range of $E = 0.1, \ldots, 10$ keV/amu for the reactions:

$$O^{8+} + H(1s) \rightarrow O^{7+*}(nl) + H^+ \quad (1)$$

$$O^{8+} + He(1s^2) \rightarrow O^{7+*}(n'l') + He^+(1s) \quad (2)$$

$$O^{8+} + He(1s^2) \rightarrow O^{6+**}(n''l'', n'''l''') + He^{2+} \quad (3)$$

using the two-state linear LZ model (for a review see the standard handbook [2]) and the modified classical OBM [1]. The calculations were made in the framework of independent particle model. In case of the He target we do not regard the autoionization process following the DEC (called ADEC channel).

In spite of the fact that for the SEC and DEC processes in collisions of multiply charged ion and light atoms the more sophisticated large scale close-coupling calculations based on the atomic orbital (AOCC) and molecular orbital (MOCC) expansion method [3] generally well reproduce the experimentally determined total and state selective cross-sections, the LZ and OBM theories have the advantage that the capture probability can be expressed analytically.

2. Calculations

We restrict the formulation to the case with one active electron with effective quantum number n_0 labeling its initial binding energy $E_0 = 1/(2n_0^2)$ on the target in a simplified collision system consisting of the target and projectile with $Z_T = 1$ and q effective charge, respectively and we start from a semiclassical treatment, assuming rectilinear trajectories for the motion of nuclei $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$ (here $\boldsymbol{R}$ is the internuclear distance, $\boldsymbol{v}$ is the impact velocity and $\boldsymbol{b}$ is the impact parameter in the centre of mass frame reference). The charge-exchange cross-sections are expressed as

$$\sigma = 2\pi \int_0^{b_{\max}} bP(b)\,\mathrm{d}b, \quad (4)$$

where P denotes the SEC or DEC probabilities calculated in the framework of LZ and OBM models and $b_{\max}$ is the width of the reaction window.

2.1. Landau–Zener model

When multiply charged ions collide with neutral atoms, a variety of electron-transfer channels are possible. The two-state LZ model is useful for the description of the electron capture process, if the transition takes place between two quasi-molecular states (formed around the approaching and receding nuclei) which are dominantly coupled at the crossing of the corresponding diabatic potential energy curves that correlate to the initial and final bound electronic states (centered on the target and projectile) in the separated atomic limits. Particularly effective transition may occur between states with the same symmetry and the same nodal structure. The most populated capture level of the final state of the projectile can be expressed by the scaling rule $n \approx 2^{1/4}q^{3/4}n_0$. The SEC probability P_{LZ} after two passages through the narrow crossing zone, using the linear model around the crossing point R_{cn}, is given by the formulas

$$P_{LZ} = 2p(1-p), \quad p(v,b) = \exp\left[-\frac{2\pi\Delta^2(R)}{v_R\Delta F(R)}\right]_{R_{cn}} \quad (5)$$

in the perturbed stationary state approximation, where Δ is the off-diagonal matrix element coupling the two interacting states. Δ is equal to half of the adiabatic energy splitting at R_{cn} between the eigenstates of the Born–Oppenheimer Hamiltonian of the one-electron diatomic molecular (OEDM) system. $v_R = v(1 - b^2/R^2)^{1/2}$ is the radial velocity and ΔF is the difference in slopes of the diabatic potential curves. The transitions are controlled by the long range forces and take place at relatively large internuclear separation. Since the crossing takes place at large internuclear separations, the pseudocrossing points can be determined approximately by using the perturbation method for the asymptotic expansion of the molecular energies and keeping the terms in them to first order (see [4]). This leads to

$$R_{cn} = \frac{2n^2(q-1)}{q^2 - (n/n_0)^2}. \tag{6}$$

The difference of the slopes between the adiabatic curves at R_{cn} can also be obtained by using the same expansion

$$\Delta F(R_{cn}) = \left|\frac{q-1}{R_{cn}^2}\right|. \tag{7}$$

For calculation of the coupling matrix element at R_{cn}, we used the following analytical formula

$$\Delta(R_{cn}) = \frac{9.13}{\sqrt{q}} \exp\{-1.324 R_{cn}/(n_0\sqrt{q})\}, \tag{8}$$

proposed by Olson and Salop [5]. This function was constructed by fit to the Δ results obtained by the numerical solution of the one-electron two-center problem for ($4 \leqslant q \leqslant 54$, e, $Z_T = 1$) cases. For the systems where the target is not atomic hydrogen the argument of the exponential function of Eq. (8) is modified by the factor n_0^{-1}.

When a low energy HCI interacts with a two-electron target, the two-electron transfer can produce an (nl, $n'l'$) double excited states of the projectile ion. In a simple approximate approach to this problem, we assume that both electrons are captured simultaneously in one step at the same R_{cn} crossing point. Thus for He target, the transition probabilities of the SEC and DEC channels can easily be calculated by means of the P^{LZ} one-electron capture probability:

$$P_{SEC,LZ}^{(He)} = 2P_{LZ}(1 - P_{LZ}) = 4p - 12p^2 + 16p^3 - 8p^4,$$
$$P_{DEC,LZ}^{(He)} = P_{LZ}^2 = 4p^2 - 8p^3 + 4p^4. \tag{9}$$

A proper treatment of the mechanism for double-electron capture producing projectile doubly excited state can be found, for example, in work [6]. Integration of the probability P^{LZ} over the impact parameter up to $b_{max} = R_{cn}$ and change of the variable b to $y = (1 - b^2/R_{cn}^2)^{-1/2}$ in Eq. (4) allow to express the total SEC cross-sections for H target in the form:

$$\sigma_{SEC,LZ}^{(H)}(v) = 4\pi R_{cn}^2 [E_3(x) - E_3(2x)], \tag{10}$$

where $E_3(x)$ is the integral:

$$E_3(x) = \int_1^\infty \frac{\exp(-xy)}{y^3}\,\mathrm{d}y \quad \text{with} \quad x = \frac{2\pi\Delta^2(R_{cn})}{v\Delta F(R_{cn})}. \tag{11}$$

We note

$$E_3(x) = \frac{1}{2}[\mathrm{e}^{-x}(1-x) + x^2 E_1(x)] \quad \text{and}$$
$$E_1(x) = Ei(-x), \tag{12}$$

where $Ei(x)$ denotes the well known integral exponential special function.

Inserting expression Eq. (9) into the integral Eq. (4) we obtain the total SEC and DEC capture cross-sections in the following forms:

$$\sigma_{SEC,LZ}^{(He)}(v) = 8\pi R_{cn}^2 [E_3(x) - 3E_3(2x) + 4E_3(3x) - 2E_3(4x)], \tag{13}$$

$$\sigma_{DEC,LZ}^{(He)}(v) = 8\pi R_{cn}^2 [E_3(2x) - 2E_3(3x) + E_3(4x)]. \tag{14}$$

2.2. Over-barrier model

The OBM is a today's version of the classical description of the electron capture. The basic idea of the model is that the electron may pass from the target to the projectile at such a sufficiently small internuclear distance denoted by R_m where the potential barrier formed by the superposition of the Coulomb fields of the projectile ion and the target core is smaller than the Stark-shifted ionization potential of the electron characterized by the principal quantum number n_0. In the modified OBM model [1] the one-electron charge-exchange probability in Eq. (4) is given by [7]

$$P_{OBM}(v,b) = 1 - \exp\left[-\frac{f_T}{T}\int_{-t_m}^{t_m} N_\Omega(t)\,\mathrm{d}t\right]. \tag{15}$$

Here

$$N_\Omega(t) = \frac{1}{2}\frac{\sqrt{q}}{(\sqrt{q}+1)^2}\left[(\sqrt{q}+1)^2 - q - R(t)/(2n_0^2)\right] \tag{16}$$

is the fraction of the electron trajectories that leads to electron capture at the time moment t.

The internuclear radius for which the potential barrier goes below the ionization potential is given by

$$R_m = 2n_0^2(\alpha\sqrt{q} + 1). \tag{17}$$

The limits of the time integration in Eq. (15) is defined by the R_m distance:

$$t_m = \frac{1}{v}\sqrt{R_m^2 - b^2}, \tag{18}$$

where f_{T} is a parameter of the theory and $T = 2\pi n_0^3$. With the analytical expression for $N_\Omega(t)$ in Eq. (16) the integration in Eq. (15) can also be performed analytically:

$$\int_{-t_m}^{t_m} N_\Omega(t)\,\mathrm{d}t = 2F\left(\frac{vt_m}{b}\right), \tag{19}$$

where

$$F(x) = \frac{\sqrt{q}}{2(\sqrt{q}+1)^2}\left[\left\{\left(\sqrt{q}+1\right)^2 - q\right\}\frac{bx}{v} - \left(\frac{b^2}{4vn_0^2}\right)\left\{x\sqrt{1+x^2} + \mathrm{arsh}(x)\right\}\right]. \tag{20}$$

In addition to the parameter f_{T}, the model contains a further parameter α that adjust the value of R_m. In our calculations we had $\alpha = 1$ and $f_{\mathrm{T}} = 2$. The SEC and DEC classical probabilities in the case of the He target can be written as

$$P_{\mathrm{SEC,OBM}}^{(\mathrm{He})} = 2P_{\mathrm{OBM}}(1 - P_{\mathrm{OBM}}), \quad P_{\mathrm{DEC,OBM}}^{(\mathrm{He})} = P_{\mathrm{OBM}}^2. \tag{21}$$

The OBM cross-sections values are obtained from Eq. (4) by numerical integration with $b_{\max} = R_m$.

3. Results

Figs. 1 and 2 show comparison of the present theoretical calculations with the experimental data of Iwai et al. [8] and Panov et al. [9], the predictions of the more realistic theory [10,11] based on a MOCC expansion method, as well as cross-sections obtained by classical trajectory Monte Carlo (CTMC) calculations [12]. We note that for He target the experimental SEC data contains con-

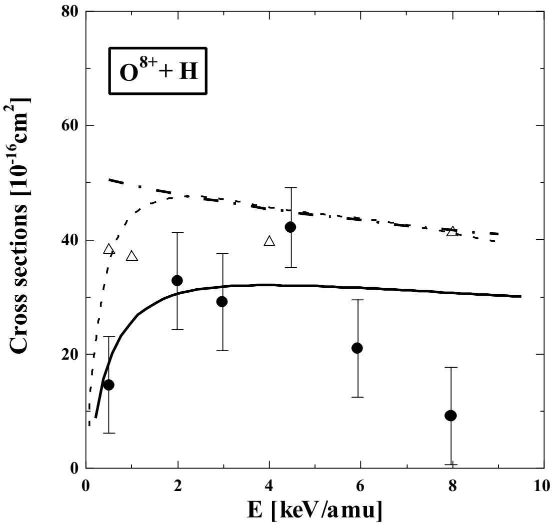

Fig. 1. Electron capture cross-sections as a function of the impact energy for the O^{8+} + H system. Theory: solid curve, LZ model; broken curve, Harel et al. [10]; open triangles, CTMC method [12]; dash-dot curve, OBM model. Experiment: closed circles, Panov et al. [9].

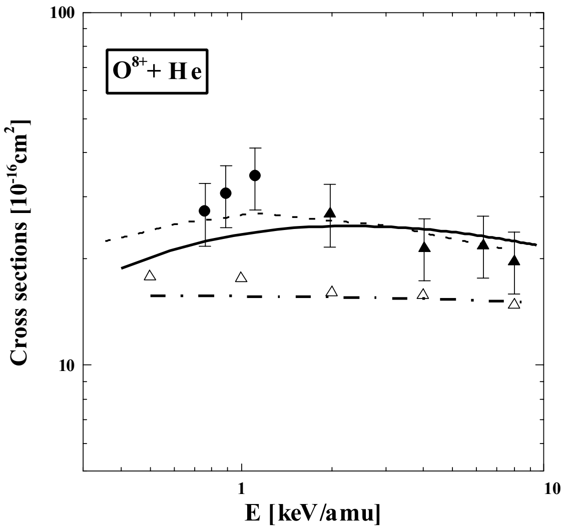

Fig. 2. Electron capture cross-sections as a function of the impact energy for the O^{8+} + He system. Theory: solid curve, LZ model (SEC + DEC); broken curve, Harel and Jouin [11] (SEC + ADEC); open triangles, CTMC method [12] (SEC + DEC); dash-dot curve, OBM model (SEC + DEC). Experiment: closed circles, Panov et al. [9] (SEC + ADEC); closed triangles, Iwai et al. [8] (SEC + ADEC).

tribution from the ADEC channel (autoionization following DEC). ADEC is not included in the present theoretical models (LZ, OBM). We took this channel into consideration by assuming that the cross-section for ADEC to a reasonable approximation is equal to the DEC cross-section.

From the figures we may conclude that although the LZ cross-sections are in better agreement with the experiment than the OBM cross-sections, the latter model is also suitable for the order-of-magnitude estimation of the charge-exchange cross-sections. The present LZ approach, which is much simpler than the MOCC methods of Harel et al. [10,11], explains more or less all the experimental features of the absolute measurement of Iwai et al. [8] and Panov et al. [9].

4. Conclusions

The results of the present work show that SEC and DEC cross-sections for collisions of low-velocity HCIs with light atoms can be calculated effectively by using simple analytical and semi-analytical theories. Particularly, we used the LZ approach and a recently developed version of the classical OBM. The fact the LZ model is in a better agreement with both the sophisticated close-coupling calculations and the experimental data than the OBM model indicates that quantum mechanical effects (formation of quasi-molecular states with various symmetries) are not negligible in the regarded collisions. Nevertheless, simple classical approaches (e.g. OBM) are suitable for fast estimation of the cross-sections.

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