

A comparative study of classical and semiclassical models of the $H^+ - Na^*(3p)$ charge exchange process

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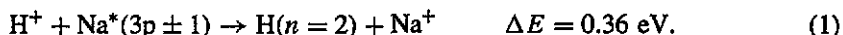
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Abstract. The electron capture process from $Na^*(3p \pm 1)$ atoms by a proton has been studied both classically and semiclassically in the energy range from 1 to 10 keV. In the classical model, we have developed a three-body classical trajectory Monte Carlo (CTMC) method with both a Coulomb potential and a model potential for the $e^- - Na^+$ interaction. In the semiclassical model, an adiabatic molecular basis including an electron translation factor is employed to describe the electronic wavefunction. When the $e^- - Na^+$ interaction is described by a model potential, at large impact parameter the CTMC probabilities are in good agreement with the semiclassical molecular probabilities at low energies and with the semiclassical atomic probabilities at higher energies.

1. Introduction

We study the charge transfer mechanism for the quasi-resonant reaction:



Our main purpose is to ascertain whether the strong orientation effect found at large impact parameters in the semiclassical molecular or atomic calculations concerning the charge transfer probabilities can be reproduced in a classical model.

We have used successively the classical trajectory Monte Carlo (CTMC) method and the semi-classical impact parameter method with a molecular basis. The CTMC method has been applied with some success in the field of intermediate energy ion–atom collisions by Abrines and Percival (1966a,b), Olson and Salop (1977) and in atom–diatom collisions by Karplus *et al* (1965). The method is based on the numerical integration of the three-body system subjected to Coulomb interactions and on a statistical distribution of the initial conditions, the problem being to know which statistics is the best to approach a quantal electronic state. Becker and MacKellar (1984) have improved the description of the atomic state using a microcanonical distribution corresponding to a given state in $|n, l\rangle$. Recently, Peach *et al* (1985) and Reinhold and Falcon (1986) have each developed more elaborate methods to replace the Coulomb interactions by a model potential for the ionic cores. In these two studies, the generation of initial electronic conditions is different. In the work of Peach *et al* (1985), the random parameters, apart from the energy and the angular momentum, are the inclination of the plane of the orbit and three action angles. In the work of Reinhold and Falcon (1986), the set of random variables are obtained by two successive transformations of a microcanonical distribution presented by Abrines and Percival (1966a), they are expressed with the momentum and position spherical coordinate angles. The CTMC

method has already been used for oriented atoms by Kohring *et al* (1983) and recently by Pascale *et al* (1990). In a recent study (Lewartowski and Courbin 1992), we have performed classical calculations for electron capture from the polarized state $\text{Na}^*(3p \pm 1)$ at 1 keV with a Coulomb interaction. We have shown a good qualitative agreement with the molecular semiclassical model and have confirmed a large orientation effect on the capture probability. We did not get exactly the same impact parameter threshold behaviour of the capture probability in our comparison of the CMTC method and the semi-classical molecular calculations (see figure 2 of this paper). The present work intends to improve the method by introducing a model potential for the $e^- - \text{Na}^+$ interaction.

We present the classical results obtained with a model potential employing the method of Reinhold and Falcon (1986) and compare them to our recent calculations using Coulomb interactions. Furthermore, the semiclassical impact parameter method with 19 molecular states has been developed for this system (Courbin *et al* 1990). The agreement of the total charge exchange cross sections from $\text{Na}(3s)$ and $\text{Na}^*(3p)$ to $\text{H}(n = 2)$ between this 19-state molecular basis, the 49-state atomic basis calculations of Fritsch (1984), the 19 (and 33) state atomic basis calculations of Dubois *et al* (1993) and the experimental cross sections measured by Royer *et al* (1988) and Richter *et al* (1990) allows us to rely upon the adiabatic molecular wavefunctions for the energy range $0.3 < E < 2$ keV. Moreover the recent measurement of the effect of the orientation on the differential cross sections (Houwer *et al* 1992) is well accounted for by this semiclassical 19-state molecular model at $E = 1$ keV and by the atomic basis calculations of Dubois *et al* (1992). At higher energy ($E > 2$ keV) we consider that the molecular expansion is no more valid and that the atomic calculations are the only reliable ones. Thus we compare the CTMC calculations with both kinds of semiclassical calculations.

We do not compare the differential cross sections as we do not expect that the CTMC model can reproduce the interference phenomena obtained in the semiclassical differential cross sections. Furthermore the experiment (Houwer *et al* 1992) and the semiclassical calculations (Dubois *et al* 1993) show that the orientation effect in the differential cross sections has nothing to do with the orientation exhibited by the probabilities. This can be expected at very small scattering angles when the phases and the deflection functions are crucial to reproduce interference phenomena. Thus we limit the comparison to the charge transfer *probabilities*. Atomic units are used throughout this paper.

2. Classical model

2.1. Dynamics

In reaction (1), we consider the three-particle collisional system composed of the incident projectile H^+ , the valence electron of sodium and the ion Na^+ . We want to simulate the geometry of the experiment (Houwer *et al* 1992) where the direction of the laser beam of circularly polarized photons (chosen as the quantization axis OZ of the electronic angular momentum) is perpendicular to the incident ion beam direction OY . We consider the collision plane which is perpendicular to OZ (see figure 1). In the present notation $\text{Na}^*(3p - 1)$ corresponds to the case where the angular momenta of the outer electron and of the incident ion (with respect to the Na nucleus) are in the same direction.

The motion of the system is determined via the Hamiltonian

$$H = \sum_{i=1}^3 \frac{p_i^2}{2m_{\text{H}^+}} + \sum_{i=4}^6 \frac{p_i^2}{2m_{e^-}} + \sum_{i=7}^9 \frac{p_i^2}{2m_{\text{Na}^+}} + V_{\text{Na}^+e^-} + V_{\text{Na}^+\text{H}^+} + V_{\text{H}^+e^-}$$

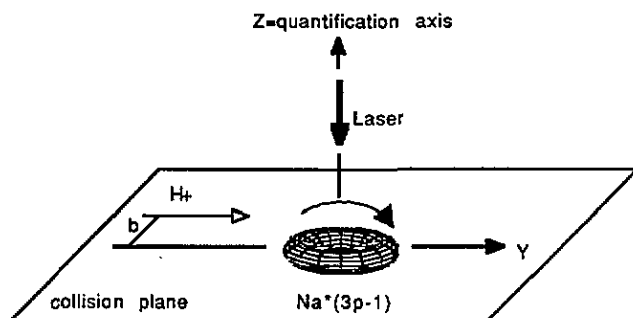


Figure 1. Scheme of the collision $\text{Na}^*(3p-1) + \text{H}^+$.

and the 18 coupled equations of motion:

$$\begin{cases} \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \\ \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \end{cases} \quad (2)$$

where p_i and q_i are the momenta and the Cartesian coordinates of the particles and V_{AB} is the interaction potential between particles A and B. The numbers of coupled equations is reduced to 12 by changing to generalized coordinates (Olson and Salop 1977). For the complete system of three particles the initial relative motion of the incident ion is specified by the asymptotic velocity along the OY axis, the asymptotic distance R and an impact parameter b .

The equations of motion are integrated until H^+ is at large distance from Na^+ , $R > 500$ au. At the end of the collision the electronic energy is computed and can be 'quantized' to yield a principal quantum number n if the energy falls within the limits

$$E(n) = \frac{-1}{2(n \pm \frac{1}{2})^2}.$$

This formula approximates the correct phase space distribution given by Becker and MacKellar (1984). Then we can define the n value of the charge transfer state $\text{H}(n)$ and especially the favoured $\text{H}(n=2)$ state in the studied reaction (1).

2.2. Initial electronic conditions for the Coulomb potential

All the interactions $V_{\text{Na}^+\text{e}^-}$, $V_{\text{Na}^+\text{H}^+}$ and $V_{\text{H}^+\text{e}^-}$ are pure Coulomb interactions. The method used is equivalent to that of Olson and Salop (1977) modified by Cohen (1982). An $|n\rangle$ state is specified by the binding energy E_0 (in the present case the binding energy of $\text{Na}(3p)$ is taken as -0.111 au) and five pseudorandom additional parameters: the eccentricity ϵ of the Kepler orbit $\epsilon^2 = 1 + 2E_0L^2$, the three Euler angles ϕ , ψ , θ fixing the plane of the orbit in space and the eccentric angle u fixing the initial position of the electron on this orbit. The parameters are distributed in the following ranges: $\epsilon^2 \in [0, 1]$; $\phi \in [-\pi, +\pi]$; $\psi \in [-\pi, +\pi]$; $\cos \theta \in [-1, +1]$; $u \in [0, +2\pi]$. The $|n, l\rangle$ state is specified by four parameters ϕ , ψ , θ and u because in this case E_0 and L are fixed for each individual trajectory. In order to determine the cross sections and transition probabilities,

one needs to choose a distribution of classical angular momenta that are restricted to the interval $l \leq L \leq l+1$ so that the square of the eccentricity is chosen in the interval: $\epsilon^2 \in [1 + 2E_0(l+1)^2, 1 + 2E_0l^2]$. In the case of the polarized atom $\text{Na}^*(3p \pm 1)$ the quantum numbers E_0, l, m are fixed. Then one random variable θ is eliminated because m is fixed, and $\cos \theta = m/[l(l+1)]^{1/2}$ takes a fixed value (Lewartowski and Courbin 1992). For the $|n, l, m\rangle$ state there are three remaining random parameters defining the electronic initial conditions: $\phi \in [-\pi, +\pi]$; $\psi \in [-\pi, +\pi]$ and $u \in [0, +2\pi]$.

If OZ is the quantification axis, the $\text{Na}^*(3p+1)$ state is characterized by $\theta = \pi/4$ and v along OY in the plane (XY) (figure 1). The $\text{Na}^*(3p-1)$ state is characterized by $\theta = 3\pi/4$ and v along OY in the plane (XY).

2.3. Initial electronic conditions for the model potential

The interactions $V_{\text{Na}^+\text{H}^+}$ and $V_{\text{H}^+\text{e}^-}$ are Coulombic and we adopt a model potential description for the $\text{e}^- - \text{Na}^+$ interaction. For compatibility with the semiclassical calculations, we adopt the same model potential. This was given in a convenient form by Klapisch (1969):

$$V(r) = -[10 \exp(-\alpha r) + \beta r \exp(-\gamma r) + 1]/r \quad (3)$$

where $\alpha = 7.902$, $\beta = 23.51$ and $\gamma = 2.688$.

The microcanonical distribution function corresponding to the active electron is given by:

$$\rho(r, p) = N \delta(E_0 - p^2/2\mu - V_L(r)) \quad (4)$$

where r and p are the position and the momentum of the active electron, N is a normalization constant, E_0 the binding energy of the active electron (-0.111 au for the $\text{Na}(3p)$ case), μ is the reduced mass of the active electron-target core system and

$$V_L(r) = V(r) + L^2/2\mu r^2 \quad (5)$$

defines the effective potential for the electron.

The electronic position coordinates are confined to the intervals where the quantity $p^2/2\mu = E_0 - V_L(r)$ keep positive values. The equation $E_0 - V_L(r) = 0$ has two roots for the considered bound state so that the variations of the variable r is restricted to the interval $r_1^L < r < r_2^L$ where r_1^L and r_2^L are those two roots. For this kind of potential the orbit is planar as in the Coulomb case and r_1^L and r_2^L define the two circles between which the precessing orbit evolves.

We perform as Reinhold and Falcon (1986) two successive changes of coordinates. First we transform these variables to a set of new variables:

$$(r, p) \rightarrow (E, r, v_r, v_p, \vartheta_r, \vartheta_p)$$

where $(r, \theta_r, \vartheta_r)$ and $(p, \theta_p, \vartheta_p)$ are the position and the momentum spherical coordinates of the active electron ($v_r = \cos \theta_r$, $v_p = \cos \theta_p$). They are defined by:

$$\begin{aligned} x &= r(1 - v_r^2)^{1/2} \cos \vartheta_r & y &= r(1 - v_r^2)^{1/2} \sin \vartheta_r & z &= r v_r \\ p_x &= \{2\mu[E - V_L(r)]\}^{1/2} (1 - v_p^2)^{1/2} \cos \vartheta_p \\ p_y &= \{2\mu[E - V_L(r)]\}^{1/2} (1 - v_p^2)^{1/2} \sin \vartheta_p \\ p_z &= \{2\mu[E - V_L(r)]\}^{1/2} v_p. \end{aligned} \quad (6)$$

The new variables are confined to the intervals $E \in (-\infty, 0)$; $r \in [r_1^L, r_2^L]$; $v_r \in [-1, 1]$; $v_p \in [-1, 1]$; $\vartheta_r \in [0, 2\pi]$; $\vartheta_p \in [0, 2\pi]$. The Jacobian of this transformation is:

$$J_1 = \mu r^2 \{2\mu[E - V_L(r)]\}^{1/2}$$

the distribution for the new variables becomes:

$$\rho(E, r, v_r, v_p, \vartheta_r, \vartheta_p) = N \mu r^2 \{2\mu[E - V_L(r)]\}^{1/2} \delta(E - E_0). \quad (7)$$

The second transformation performed is:

$$(E, r, v_r, v_p, \vartheta_r, \vartheta_p) \rightarrow (E, \omega, v_r, v_p, \vartheta_r, \vartheta_p).$$

The variable ω is defined by:

$$\omega(r) = \int_{r_1^L}^r dr' \mu r'^2 \{2\mu[E_0 - V_L(r')]\}^{1/2}. \quad (8)$$

The domain for the new parameter ω is such that $\omega \in [0, \omega(r_2^L)]$ when $r \in [r_1^L, r_2^L]$. The Jacobian of this transformation is:

$$J_2 = \frac{dr}{d\omega} = \mu^{-1} r^{-2} \{2\mu[E_0 - V_L(r)]\}^{-1/2}. \quad (9)$$

The probability density in terms of the new coordinates becomes:

$$\rho(E, \omega, v_r, v_p, \vartheta_r, \vartheta_p) = N \delta(E - E_0)$$

as desired and initial conditions can be easily generated.

For a $|n, l\rangle$ state the classical value L is chosen restricted to $l \leq L \leq l+1$. When L is fixed the parameter ω is uniformly distributed in the interval $[0, \omega(r_2^L)]$ and so we restrict the value of r to $r \in [r_1^L, r_2^L]$. The variable ω defines the initial value of r of the electron. It remains to define the direction of the orbital plane (or the L direction). This direction is defined by the parameters $v_r, v_p, \vartheta_r, \vartheta_p$ which fix respectively the directions of the initial r and p vectors. The variables $v_r, v_p, \vartheta_r, \vartheta_p$ are chosen randomly from the corresponding intervals: $v_r \in [-1, 1]$; $v_p \in [-1, 1]$; $\vartheta_r \in [0, 2\pi]$; $\vartheta_p \in [0, 2\pi]$ but the values of ϑ_r and ϑ_p are restricted so that the relation:

$$|L| = |r \wedge p| \quad (10)$$

linking v_r, v_p, ϑ_r and ϑ_p to the fixed value L is fulfilled. So those four numbers are reduced, because of relation (10), to three numbers which are normally required to define a plane in a three-dimensional space. Practically for a choice of v_r, v_p the random values of ϑ_r, ϑ_p are kept as initial conditions only if they correspond to values compatible with the relation (10).

For a $|n, l, m\rangle$ state, added to the relation (10) we fix now the L_Z value such that $L_Z = m = \pm 1$:

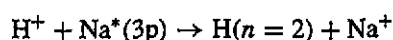
$$\pm 1 = r \{2\mu(E_0 - V_L)\}^{1/2} (1 - v_r^2)^{1/2} (1 - v_p^2)^{1/2} \sin(\vartheta_p - \vartheta_r). \quad (11)$$

Equations (10) and (11) relate the four parameters v_r, v_p and ϑ_p, ϑ_r so that only two free parameters remain. For the full initial condition problem the random value ω is the other parameter and we have three parameters to describe a $|n, l, m\rangle$ state as it should be. Practically the condition $1 \leq L < 2$ leads to values of the parameter $v_r = \cos \theta_r$ such that $|v_r| < \sqrt{2}/2$. The same condition applied for v_p . These two parameters are chosen randomly in the interval $(-\sqrt{2}/2, \sqrt{2}/2)$, and we keep the values of v_r, v_p which are compatible with the relations (10) and (11), then we choose a random parameter $\vartheta_p \in [0, 2\pi]$ and ϑ_r is directly determined by equation (11). The parameter ϑ_p plays the role of the ϕ angle of the Coulomb case (section 2.2).

2.4. Numerical method

Two different numerical methods have been used to solve the 12 coupled equations (2): a fourth-order Runge–Kutta method with an adaptative step-size control and the method of Bulirsch and Stoer (1966). With the Runge–Kutta method 50 trajectories were computed in 1 h on an IBM 3090 with four parallel processors. The use of the method of Bulirsch and Stoer increases the speed by a factor of 30. This permits an easier study of reaction (1) for different energies and different interactions. By increasing the number of trajectories calculated for each impact parameter, we have diminished the RMS standard deviation errors compared to the previous study (Lewartowski and Courbin 1992). The errors are smaller than 5%.

As a test of our CTMC program with a model potential we have calculated total charge exchange cross sections for the following reaction:



where the Na^* atom is not polarized. We have compared our results with the molecular calculations of Courbin *et al* (1990), the atomic calculations of Fritsch (1988), the atomic calculations of Dubois *et al* (1993) and the experimental results of Richter *et al* (1990). The total charge exchange cross section obtained from the semiclassical data is such that each of the three components of the $\text{Na}^*(3p)$ state are initially equally populated and is given by:

$$\sigma_{\text{Na}^*(3p) \rightarrow \text{H}(n=2)} = \frac{1}{3}(\sigma_{\text{Na}(3p\Sigma) \rightarrow \text{H}(n=2)} + \sigma_{\text{Na}(3p\Pi^+) \rightarrow \text{H}(n=2)} + \sigma_{\text{Na}(3p\Pi^-) \rightarrow \text{H}(n=2)}).$$

The results presented in table 1 will be discussed in section 4.

Table 1. Comparison of $\text{H}^+ + \text{Na}^*(3p) \rightarrow \text{H}(n=2) + \text{Na}^+$ charge transfer cross sections (in \AA^2): a, CTMC calculations with Coulombic potential; b, CTMC calculations with model potential; c, semiclassical molecular calculations of Courbin *et al* (1990); d, semiclassical atomic calculations of Fritsch (1988); e, semiclassical atomic calculations of Dubois *et al* (1992); f, experimental results of Richter *et al* (1990).

E_{lab} (keV)	a	b	c	d	e	f
1	$47.2 \pm 8\%$	$72 \pm 7\%$	74.0	64.4	69.9	92.3^\dagger
2	$41.5 \pm 9\%$	$59.1 \pm 5\%$	64.6	60.1^\dagger	56.7	57.2^\dagger
5	$27.9 \pm 9\%$	$27.2 \pm 6\%$	47.9	27.1	24.2	
8	$20.8 \pm 10\%$	$17.4 \pm 7\%$		12.1		

† Values corresponding to $E_{\text{lab}} = 1.7$ keV.

‡ These values are calibrated on the charge transfer cross section $\sigma_{\text{Na}(3s) \rightarrow \text{H}(n=2)}$ calculated by Courbin *et al*.

3. Semiclassical molecular model

When the relative velocity of the collision partners is low compared with the classical velocity of a bound electron in a Bohr orbit, the electronic Hamiltonian H_{el} can be approximated in the adiabatic representation. At the considered intermediate energies, we have employed the semiclassical impact parameter model for nuclear motion and developed

the wavefunction $\Psi(\mathbf{r}, t)$ on a basis set of adiabatic molecular wavefunctions $\chi_n(\mathbf{r}, R)$ defined by

$$H_{\text{el}}\chi_n(\mathbf{r}, R) = \epsilon_n\chi_n(\mathbf{r}, R)$$

where H_{el} is developed using a model potential method (Valiron 1973).

As a purely adiabatic basis does not reproduce the dragging effect on the electron of the motion of the nuclei and introduces unrealistic effects at asymptotic distances, the molecular basis set is modified by an electronic common translation factor (CTF) g . Then expanding $\Psi(\mathbf{r}, t)$ in the form

$$\begin{aligned}\Psi^{\text{CTF}}(\mathbf{r}, t) &= \exp\{ig(\mathbf{r}, R)\} \sum_{n=1}^N c_n(t)\chi_n(\mathbf{r}, t) \exp\left(-i \int_0^t \epsilon_n(R(t'))dt'\right) \\ &= \sum_{n=1}^N a_n(t)\chi_n^{\text{CTF}}(\mathbf{r}, t)\end{aligned}$$

one obtains from application of the time-dependent Schrödinger equation, the set of coupled equations for the coefficients $a_n(t)$:

$$i \frac{\partial a_n}{\partial t} = \sum_m a_m V_{nm}^{\text{CTF}} \quad (12)$$

where

$$V_{nm}^{\text{CTF}} = \langle \chi_n^{\text{CTF}} | \epsilon_n - \partial/\partial t | \chi_m^{\text{CTF}} \rangle$$

defines the coupling matrix elements.

The electronic common translation factor is

$$g(\mathbf{r}, R) = f(\mathbf{r}, R)\mathbf{v} \cdot \mathbf{r} - \frac{1}{2}f^2(\mathbf{r}, R)v^2t$$

with

$$f(\mathbf{r}, R) = (1/R)y \quad \text{and} \quad y = \mathbf{R} \cdot \mathbf{r}.$$

Equations (12) have been solved numerically for a particular impact parameter b and for a given molecular basis set. The molecular basis is described by Allan (1986) in whose work the model potential method is applied. The model potential to describe the e^- - Na^+ interaction is the Klapisch potential given in equation (3), as in the preceding classical method. We treat the problem with a basis including 19 molecular states $\text{Na}(3s\Sigma, 3p\Sigma, 3p\Pi^\pm, 4s\Sigma, 3d\Sigma, 3d\Pi^\pm, 4p\Sigma)$ and $\text{H}(2\sigma^+, 2\sigma^-, 2p\Pi^\pm, 3p\Sigma^\pm, 3p\Pi^\pm, 3d\Sigma, 3d\Pi^\pm)$ where σ^+ and σ^- denote the two hybrid bonding and antibonding states (Courbin *et al* 1990).

We consider collisions involving capture of the outer electron of sodium into the $\text{H}(n=2)$ states. Consequently we must include the coupling due to the Stark effect $\langle \chi_n | H_{\text{Stark}} | \chi_m \rangle$ in the evolution matrix U . The Stark effect is induced by the alkali ion Na^+ in the field of the two degenerate states $\text{H}(2s)$ and $\text{H}(2p)$.

The circularly polarized states $\text{Na}^*(3p \pm 1)$ are quantized along the OZ axis. These states are complex states and can be expressed as a combination of the real molecular states:

$$|3p \pm 1\rangle = \pm(-|3p\Sigma\rangle \mp i|3p\Pi^+\rangle)/\sqrt{2}.$$

The corresponding S -matrix elements for this type of initial state are:

$$S_{j,3p\pm 1} = \pm\{-S_{j,3p\Sigma} \mp iS_{j,3p\Pi^+}\}/\sqrt{2} \quad (13)$$

and the corresponding probabilities can be deduced:

$$P_{j,3p\pm 1} = \{|S_{j,3p\Sigma}|^2 + |S_{j,3p\Pi^+}|^2 \pm 2\text{Im}(S_{j,3p\Sigma}S_{j,3p\Pi^+}^*)\}/2. \quad (14)$$

The following probabilities $P_{\text{Na}(3p\Sigma) \rightarrow \text{H}(n=2)}$, $P_{\text{Na}(3p\Pi^+) \rightarrow \text{H}(n=2)}$, $P_{\text{Na}(3p\Pi^-) \rightarrow \text{H}(n=2)}$ and consequently $P_{\text{Na}(3p\pm 1) \rightarrow \text{H}(n=2)}$ can be computed as a function of impact parameter.

4. Results and discussion

The relative collision energy range explored is 1–10 keV. As the velocity of the electron in the $\text{Na}^*(3p)$ orbit is approximatively $v_{e^-} = 0.47$ au, the relative collision velocity range studied is $0.42 \leq v_{\text{H}^+}/v_{e^-} \leq 1.4$, where v_{H^+} is the velocity of the incident proton.

In table 1 are presented the total charge exchange cross sections for the reaction $\text{H}^+ + \text{Na}^*(3p) \rightarrow \text{H}(n=2) + \text{Na}^+$ calculated by different methods and the experimental results. Firstly we notice the very good agreement at all the considered energies between the model potential classical calculations and the two semiclassical calculations with a large atomic basis (Fritsch and Dubois *et al.*). The classical Coulomb calculations give too small cross sections at 1 and 2 keV and too big cross sections at 8 keV. It seems that the introduction of a model potential in the CTMC method improves significantly the charge transfer cross section at the considered energies. Secondly, we remark that the molecular calculation agrees with the atomic calculations and the CTMC model potential calculations at low energies (1 and 2 keV) but not at 5 keV which is known to be outside the validity range of the molecular model. We note that the agreement with experiment is fairly good, apart from at 1 keV where the experimental value is bigger than any theoretical predictions and this remains unexplained.

In figures 2(a)–(d) we have considered reaction (1) using the CTMC method with a Coulomb potential. At all the energies the orientation effect is similar to the effect previously found at 1 keV (Lewartowski and Courbin 1992). The electron is transferred preferentially when it has an angular momentum of the same sign as the adjacent ion. We note a maximum of the gap between $P_{\text{Na}(3p-1) \rightarrow \text{H}(n=2)}$ and $P_{\text{Na}(3p+1) \rightarrow \text{H}(n=2)}$ at 5 keV, which corresponds to the velocity matching where the projectile and the active electron have the same speed.

In figures 2(e)–(h) we have considered reaction (1) using the CTMC method with the Klapisch model potential introduced for the electron– Na^+ interaction. The orientation effect is still visible at all the energies. Compared to the Coulomb case, the model potential as it is more attractive shifts the probabilities to larger impact parameters, especially $P_{\text{Na}(3p+1) \rightarrow \text{H}(n=2)}$.

In figures 2(i)–(l) semiclassical results are presented for reaction (1). At all energies we observe a remarkable orientation effect, especially in the long-range interaction region at $b > 10$ au. For the initial state $\text{Na}^*(3p+1)$ the exchange processes take place between 5 and 10 au and for the $\text{Na}^*(3p-1)$ initial state it takes place between 10 and 20 au, at 1

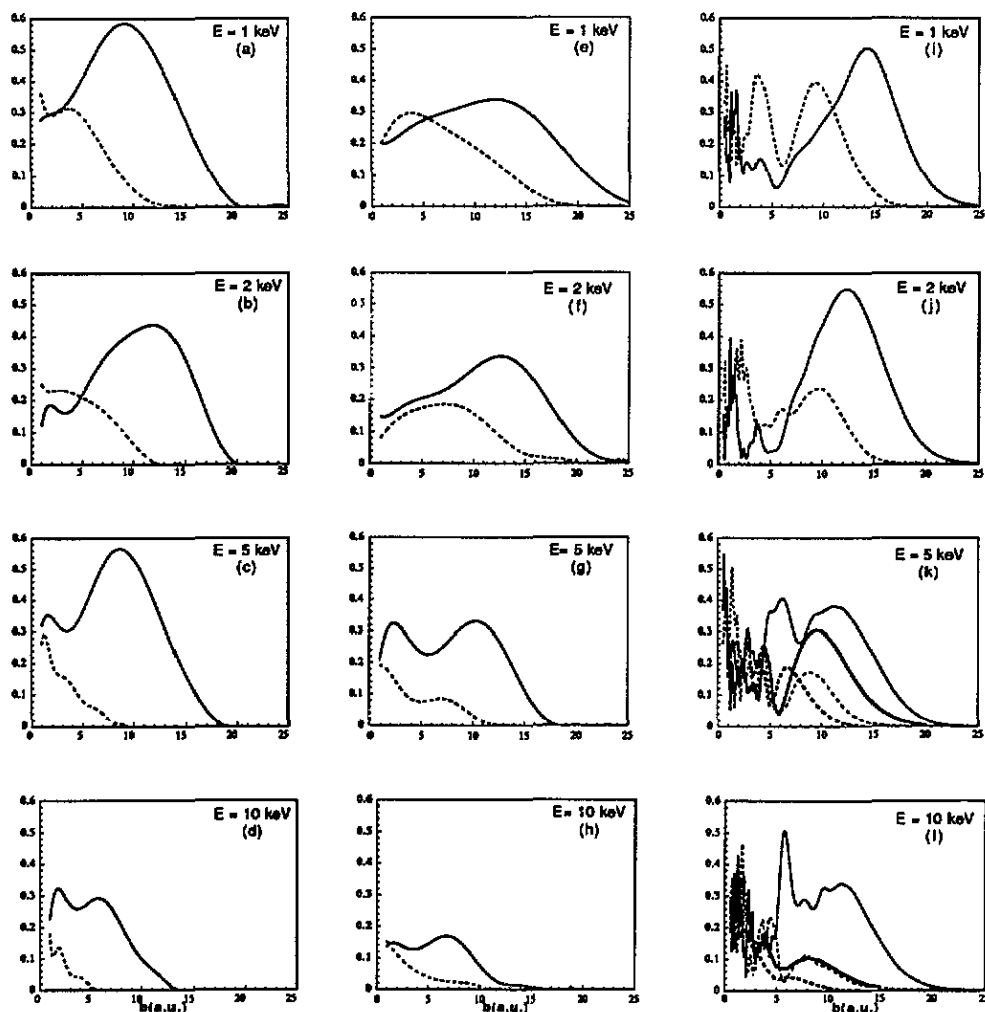


Figure 2. CTMC charge transfer probability with a Coulomb potential: (a)–(d), CTMC charge transfer probability with a model potential: (e)–(h), — $\text{Na}^*(3p-1)$; --- $\text{Na}^*(3p+1)$ initial state. Semiclassical charge transfer probability: (i)–(l), — $\text{Na}^*(3p-1)$, --- $\text{Na}^*(3p+1)$: 19 molecular states (present results). (k)–(l), — $\text{Na}^*(3p-1)$, --- $\text{Na}^*(3p+1)$: 19 atomic states at 5 keV and 33 atomic states at 10 keV (Dubois *et al.*).

and 2 keV. This strong orientation effect at large impact parameter may be understood in terms of the coupling between the three molecular states $\text{Na}(3p\Sigma)$, $\text{Na}(3p\Pi)$ and $\text{H}(2\sigma^+)$ and has already been discussed (Courbin *et al.* 1993).

A good qualitative agreement exists between the model potential classical calculations and the semiclassical molecular calculations at 1 and 2 keV (figures 2(e), (f), (i), (j)). At all the energies the orientation effect is found (even if it is not as marked compared to the Coulomb potential). The maxima and minima of amplitudes are in the same zone of impact parameters. The onset of the probabilities occurs at similar impact parameters, which is an improvement compared to the CTMC Coulomb calculations. The total cross sections are especially dependent on the probabilities at large impact parameters and this explains why a

similar behaviour of the probabilities at large impact parameters lead to similar total charge exchange cross sections (CTMC model potential and semiclassical results in table 1), even if the probabilities are different at smaller impact parameters.

At 5 keV, the molecular cross section for the unpolarized atom $\text{Na}^*(3p)$ is too big (table 1). The amplitude of the charge exchange probability is also too big for the polarized atom $\text{Na}^*(3p \pm 1)$. We know that this energy ($v_{H^+}/v_{e^-} \approx 1$) is outside the validity limit of the adiabatic molecular regime. For the energies above 5 keV, the model potential CTMC calculations must be compared with the atomic semiclassical calculations (figures 2(g), 2(h), 2(k), 2(l) with bold lines) and we can notice the good agreement.

5. Conclusion

We have obtained the total CTMC cross sections for charge transfer to $\text{H}(n = 2)$ from $\text{Na}^*(3p)$ atoms in the energy range 1–10 keV with a Coulomb and a model potential for the $e^- - \text{Na}^+$ interaction. The semiclassical results (atomic or molecular calculations) agree well with the model potential calculations regarding the charge exchange total cross sections. The model potential replacing the Coulomb potential improves the classical model of the $\text{Na}^*(3p)$ atomic state.

We have tested the effect of the model potential on the charge exchange probability to $\text{H}(n = 2)$ from $\text{Na}^*(3p \pm 1)$. The orientation effect observed in the semiclassical theory is fairly well reproduced: *in the large impact parameter range the transfer is much bigger when the electron has an angular momentum of the same sign as the adjacent ion*. The model potential for the $e^- - \text{Na}^+$ interaction improves the description of the collisional system state at all the considered collision velocities. The influence of the orientation on the capture process is demonstrated by this study of the charge transfer probability.

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