An easy method to estimate charge-exchange cross sections between ions and one-active-electron atoms

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In this paper we present a simple model for computing single electron exchange between light nuclei. The electronic capture is pictured as a tunnelling process in a model potential. This allows to analytically compute the transmission probability. Some comparisons with data from existing literature are given.

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I. INTRODUCTION

Charge exchange processes between atomic particles are of great importance in plasma physics and astrophysics. By example, it is through this mechanism that energetic charged particles can escape from the core of magnetic confinement devices; conversely, cold neutral particles coming from the wall can diffuse towards the centre. While only quantum mechanical methods can give really accurate computations of all of the basic quantities for these processes, i.e. total and partial or differential cross sections, less precise but simpler methods can still be useful. In some cases they can still give high-precision estimates. It is the case of the Classical Trajectory Monte Carlo (CTMC) method, successfully applied to high-velocity collisions (but recently extended also to the low velocity range, see, e.g., [1, 2] for a discussion and some recent improvements on this subject), to Rydberg-atom collisions, and to multiply-charged nuclei. In the low-velocity region, analytical or semi-analytical methods are often used: we mention here just the Over Barrier Models (OBMs). They are known since a long time [3] and are still being improved to include as much physics as possible [4, 5, 6, 7, 8].

It is worthwhile to notice that, although the computation of charge exchange cross sections is a well developed field of research since several decades, its techniques are by no means completely established: it may still happen that theoretical predictions be confuted by experiments or that different methods give sharp discrepancies even in relatively simple situations, that should be quite well diagnosed by now [9]. Therefore, the development of new, different methods of computation can still be valuable. In this work we suggest a fast algorithm to estimate single electron captures. From the tests that we show in this paper, it appears also rather accurate. It is rooted upon standard OBMs, in that the electronic capture process is regarded as a potential barrier crossing. Unlike OBMs, however, the electron is considered as a quantum-mechanical object. This allows to compute also under-barrier crossing events (tunnelling). In order to reduce the problem to a manageable, semi-analytical form, several geometrical simplifications will be done. The results are compared against experimental data as well as other different theoretical computations, and are found to fit them nicely.

II. DESCRIPTION OF THE MODEL

We consider a scattering experiment between a nucleus $T$ with one active electron $e$, and a projectile nucleus $P$. Let $\rho$ be the electron position relative to $T$ and $R$ the relative distance between $T$ and $P$ (see Fig. 1). Several approximations are necessary: I) All the nuclei are regarded as hydrogenlike particles, thus $Z_p$ and $Z_t$ are the effective charge of the projectile and of the target seen by the electron, respectively; II) The two nuclei are considered as approaching slowly if compared to the orbital electron velocity (adiabatic approximation). This means that the electron is allowed to complete its path from the target to the projectile before any appreciable relative movement of the nuclei occurs. III) We adopt a straight-line approximation for the nuclear trajectory. IV) We neglect the possibility of target or projectile ionization. V) Finally, we discard also the possibility of electronic re-capture from the projectile by the target (although this possibility can be implemented within the algorithm without much effort).

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Points II) and III) are not mutually contradictory provided that impact velocity $u$ is not too small. We remind that the high- and low-velocity ranges are discriminated by $u \geq v_e, u \leq v_e$, with $v_e$ classical velocity of the electron. Point IV), too, is consistent only with slow collisions. Point V), finally, is likely to be more and more satisfied as the ratio $Z_p/Z_t$ increases well beyond the unity.

Let us for a while look at the electron as it were a classical particle, and assume that it is initially in a low angular momentum state (e.g. an $s$ state): this means that its trajectory is a straight segment along the radial direction, starting from the target nucleus (Fig. 1).

The total energy of the electron is

$$E = \frac{p^2}{2} + U = \frac{p^2}{2} - \frac{Z_t}{\rho} - \frac{Z_t}{R - \rho}$$  \hspace{1cm} (1)

(Atomic units will be used unless otherwise stated). It is straightforward to work out the value and the position of the maximum of the potential $U$ along the internuclear axis, as depicted in Fig. 2:

$$U_M(\rho_M) = -\frac{1}{R} \left( \sqrt{Z_t} + \sqrt{Z_p} \right)^2,$$  \hspace{1cm} (2)

$$\rho_M = \frac{R}{\sqrt{Z_t} + \sqrt{Z_p}}.$$  \hspace{1cm} (3)

We make the hypothesis that only nearly head-on collisions of the electron on the projectile lead to capture: that is, captures occur only along or close to the internuclear axis. Let us define $p_c$ as the probability for an electron impinging exactly along this axis to be captured, and write the capture probability $f$ for electrons impinging within the solid angle $d\Omega = \sin(\xi)d\xi d\varphi$ around the internuclear axis as

$$f = p_c \delta(\varphi) \frac{d\Omega}{4\pi},$$  \hspace{1cm} (4)

where $\delta$ is the Dirac delta and $4\pi$ is a normalization factor accounting for an isotropic distribution of the electronic velocities. The presence of the delta function means that only electrons whose trajectories are completely lying in the same plane as the three particles are allowed to be captured.
FIG. 2: Potential \( U \) along the internuclear axis.

Because of the straight-line trajectory there is a one-to-one correspondence between time and angle \( \xi \):

\[
\xi = \arcsin \left( \frac{b}{R(t)} \right), \tag{5}
\]

\[
R(t) = \sqrt{b^2 + (ut)^2}, \tag{6}
\]

where \( b \) is the impact parameter.

Let us now define \( W \) as the probability for the electron to be still bound to \( T \) at time \( t \). Its rate of change as given by

\[
\begin{align*}
\frac{dW(t)}{dt} &= -fW(t) = -W(t)p_c\delta(\varphi)\frac{d\Omega}{4\pi}. \tag{7}
\end{align*}
\]

The integration over the azimuthal angle \( \varphi \) is straightforward, and we find

\[
\begin{align*}
\frac{dW(t)}{dt} &= -W(t)p_c\frac{4\pi}{\sin(\xi(t))}\frac{d\xi(t)}{dt}dt. \tag{8}
\end{align*}
\]

Integration over time, with the boundary condition \( W(-\infty) = 1 \), yields

\[
W(t) = \exp \left( -\frac{1}{4\pi} \int_{-\infty}^{t} p_c(\tau) \sin(\xi(\tau)) \frac{d\xi(\tau)}{d\tau} d\tau \right) \tag{9}
\]

and we have put into evidence that the factor \( p_c \) is a function of distance \( R \) and thus of time.

The total capture probability is \( P(b) = 1 - W(\infty) \) and the total cross section is given by the integral of this quantity in the impact parameter space: \( \sigma = 2\pi \int bP(b) db \).

By reducing everything to one-dimensional geometry, we have chosen to place all of the important physics in the transmission factor \( p_c \): the probability for an electron to cross the potential barrier. This is at a difference with, e.g.,
OBMs, where the spatial form of the potential is of critical importance (see §§§). If we choose to maintain the classical picture for the electron, we could recover a very simplified version of Over Barrier Model, by putting \( p_e = 1 \) in the region classically allowed to the electron, and zero elsewhere. We instead choose to compute \( p_e \) through a quantum-mechanical picture: we model the process of transferring the electron from one nucleus to the other as a tunnelling process through the potential barrier, with the factor \( p_e \) which becomes the transmission factor. Even for this simplified problem the quantum mechanical transmission factor can be computed only by complicated numerical techniques. Since the goal of this paper is to write down an algorithm as much simplified as possible, we shall replace the true potential with a carefully chosen model one: we use here a simple square barrier potential. One has to imagine the two nuclei to be placed externally to the barrier, on the two opposite sides of it. The transmission factor for a particle coming, say, from the left with momentum asymptotically equal to \( k_l \) is

\[
p_e = \frac{\exp[-(i/2)L(k_l - 2q + k_r)]4k_lq}{(k_l((q + k_r) + \exp[2iLq](q - k_r)) + q(q + k_r) - \exp[2iLq](q - k_r)))^2}
\]

(10)

The coefficients \( q, k_r \) are the momenta respectively within the barrier and on the right side; \( L \) is the barrier width. The momentum \( k_l \) is obviously related to the momentum of the bound electron: if its binding energy is \( -E_n \), then an intuitive choice is to set \( k_l = \sqrt{2|E_n|} \). We choose to consider energy-conserving collisions, thus we set \( k_r = k_l \). In the original problem (Fig. 2), the energy needed by the electron to reach the top of the potential hill is \( \Delta E = U_M - E_n = -|U_M| + |E_n| \). We define the height of the square potential barrier \( V_0 \) by keeping constant and equal to \( \Delta E \) the energy deficit between potential and kinetic energy: this means

\[
V_0 - \frac{k_l^2}{2} = \Delta E = -|U_M| + |E_n| \rightarrow V_0 = 2|E_n| + \frac{1}{R} \left( \sqrt{Z_l} + \sqrt{Z_p} \right)^2
\]

(11)

(where we have used Eq. [3]). This relation defines \( q \). Finally, it is clear that the barrier width \( L \) must be related to the internuclear distance \( R \): we wish to have a zero-potential region \( (V \approx 0) \) close to either of the nuclei. Basing upon indetermination relations, an electron bound to one nucleus, with kinetic energy \( k_l^2/2 \), moves within a region of spatial extent \( \Delta \approx 1/k_l \). We choose this as the width of the potential-free region and set therefore \( L = R - 2\Delta \). Of course, one must also set \( L = 0 \) when \( R < 2\Delta \). Some tests showed that only minor differences are found if \( L \) is allowed to vary slightly. For example, results shown in the next section remain almost unvaried by using the simpler choice \( L = R \).

The problem is, at this stage, reduced to performing a double integration: one over time for computing \( P(b) \), and the other one over \( b \) for getting \( \sigma \). Neither of the two quadratures can be done analytically; however, they can be performed rather easily by using any standard mathematical software package.

III. NUMERICAL RESULTS

We benchmark the model against experimental results from ref. [10] and the theoretical ones coming from the molecular approach simulation of ref. [11]. In Fig. (3) we show some typical results for impacts between multicharged hydrogen-like ions and ground state hydrogen. In all cases, impact velocity is about 1/2 a.u. (it is exactly this value for the numerical results, while in experiments 0.49 \( \leq u \leq 0.51 \)). The agreement is fairly good, with our model yielding a slight underestimate of theoretical results, but the accordance with experiment is pretty nice. The only exception is the \( Z = 10 \) case but, there, it is probable that is the experimental value to be flawed, since it departs rather abruptly from the general trend.

Tests carried out also for different velocities yielded results of comparable accuracy, with some caveat: see next section.

IV. DISCUSSION

Besides being a very simple model to implement, and still being apparently rather accurate, a remarkable feature of this model is that it is self-consistent: although the parameters \( L, V_0, k_l, \ldots \), have been guessed on the basis of order-of-magnitude reasonings, none of them is left to the experiment. However, the choice of the model potential has been arbitrary, constrained only by the condition that it must provide analytical expressions for \( p_e \). One could, therefore, wonder if even better results can be got from a different choice of the model potential. The only other such potential we are aware of is the Eckart potential [12]: it is an approximately bell-shaped potential, and therefore rather different from the curve of Fig. 2. It has, however, the advantage of being smooth, without unphysical discontinuities. We have done a few tests using it: on the whole, we did find—not surprisingly—a worsening of the performances of the
algorithm.
A discussion is, of course, necessary about the range of validity of the algorithm. First of all, care must be taken when trying to apply this model to different velocity regimes: at very low velocity $u << 1$ the straight-line approximation for nuclear motion fails. More important, according to a Feynman-like picture, the electron has more time to “sample” non-rectilinear paths connecting the two nuclei, thus making less correct the reasoning that here yielded to estimate $p_c$. For high-$u$ (say, $u \geq 1$), instead, ionization becomes relevant and the adiabatic hypothesis breaks down.

Besides the impact velocity, $\sigma$ has a functional dependence upon a number of other parameters, e.g., projectile charge $Z_p$. It is straightforward to recover from Fig. 3 a power-law behaviour for this parameter: $\sigma$ is well fitted by a second-order polynomial. Roughly speaking, a $Z_p^2$ contribution comes from $p_c$, and another one from the effective range of interaction. This functional dependence is stronger that that usually quoted in literature (which is closer to $Z_p^1$) [13]. This could cause some trouble when trying to study highly-charged-ion collisions.

[1] M.J. Raković, D.R. Schultz, P.C. Stancil and R.K. Janev, J. Phys. A: Math. Gen. 34 (2001) 4753.
[2] D.R. Schultz, P.C. Stancil and M.J. Raković, J. Phys. B: At. Mol. Opt. Phys. 34 (2001) 2739.
[3] H. Ryufuku, K. Sasaki and T. Watanabe, Phys. Rev. A 21 (1980) 745.
[4] A. Niehaus, J. Phys. B: At. Mol. Phys. 19 (1986) 2925.
[5] V.N. Ostrovsky, J. Phys. B: At. Mol. Opt. Phys. 28 (1995) 3901.
[6] F. Sattin, J. Phys. B: At. Mol. Opt. Phys. 33 (2000) 861, 2377.
[7] F. Sattin, Phys. Rev. A 62 (2000) 042711.
[8] F. Sattin, Phys. Rev. A 64 (2001) 034704.
[9] J. Caillar, A. Dubois, and J. P. Hansen, J. Phys. B: At. Mol. Opt. Phys. 33 (2000) L715.
[10] F.W. Meyer, A.M. Howald, C.C. Havener and R.A. Phaneuf, Phys. Rev. A 32 (1985) 3310.
[11] C. Harel, H. Jouin and B. Pons B, At. Data Nucl. Data Tables 68 (1998) 279.
[12] C. Eckart, Phys. Rev. 35 (1930) 1303.
[13] R.K. Janev, Phys. Lett. A 160 (1991) 67.