A Distorted Wave T-Matrix Approach to Ionization of Atoms by Slow Heavy Particle Impact

Kh.Tsookhuu and J.Madsen

Abstract

We propose a theory for the description of slow inelastic collisions between charged particles and simple atomic systems based on a T-matrix approach. Using an eikonal distortion to describe the heavy particle motion, the T--matrix is obtained by the stationary phase approximation. In result, the ionization cross section is expressed by the product between the width of decay of the "quasimolecular" system formed during the collision and a surviving probability of the heavy particle in elastic channel.

1 Introduction

The study of slow collisions of heavy particles with atoms has many physical and chemical applications. But the theoretical description of slow collisions is complicated due to inaccessibility of standard perturbation theory since the projectile velocity is smaller than the Bohr velocity.

Over the last years, in connection mainly with mesic--atom processes and muon catalyzed fusion, several methods have been developed to describe slow collisions of negative particles (muons and hadrons) with simple atoms:diabatic state [1], classical-trajectory Monte-Carlo [2], classical-quantal coupling [3], and coupled-channels semiclassical approximation [4,5]. However, none of these methods have been formulated in a general enough

framework to extend their applicability to a large range of experimental conditions.

In this paper we propose a more general theory for ionization of atoms by slow impact of charged particles based on a distorted wave T-matrix approach. Previously a T-matrix approach has mainly been utilized to describe fast and intermediate collisions [6,7].

The paper is organized as follow: in section 2 we derive the impact parameter representation of the T-matrix. In section 3 the distorted waves and perturbations are derived in two different cases: one using a molecular and one using an atomic basis for the electronic wave function in the initial state. Continuing in section 4 we use a stationary phase approximation valid at slow projectile velocities to derive a closed form of the transition matrix for slow negative projectile impact. Atomic units will be used throughout unless otherwise noticed.

2 The impact parameter representation of the T-matrix

The prior form of the transition matrix for electron emission in ion-atom collisions, in the distorted wave formulation, may be written as

$$T_{fi} = < \Psi_f^-(\mathbf{r}_T, \mathbf{R}_T)|W_i|\Phi_i^+(\mathbf{r}_T, \mathbf{R}_T) > + T^D \qquad (1)$$

where $\Psi_f^-(\mathbf{r}_T, \mathbf{R}_T)$ is the exact scattering state compatible with the considered final channel, and W_i is the perturbation in the initial channel given by

$$W_i|\Phi_i^+(\mathbf{r}_T, \mathbf{R}_T) >= \{E - H\}|\Phi_i^+(\mathbf{r}_T, \mathbf{R}_T) > . \qquad (2)$$

The second term, T^D, is the surface term which is normally considered small in ion-atom collisions (in the D2C theory [7] it may be show to vanish explicitly due to orthogonal between the initial and final electronic states). Describing the heavy particles in the final channel as $\varphi_{\mathbf{K}_f}(\mathbf{R}_T)D^-_{\mathbf{K}_f}(\mathbf{R}_T)$, where $D^-_{\mathbf{K}_f}(\mathbf{R}_T)$ is a elastic-channel distortion factor and $\varphi_{\mathbf{K}_i}(\mathbf{R}_T)$ is a plane wave, we may write the final channel wave function in the following form:

$$\Psi_f^-(\mathbf{r}_T, \mathbf{R}_T) = \psi^-_{\mathbf{k}_T}\varphi_{\mathbf{K}_f}(\mathbf{R}_T)D^-_{\mathbf{K}_f}(\mathbf{R}_T), \qquad (3)$$

where $\psi^-_{\mathbf{k}_T}$ is the electronic part of the final wave function. The corresponding T-matrix is now given by

$$T_{fi} = < \psi^-_{\mathbf{k}_T} \varphi_{\mathbf{K}_f}(\mathbf{R}_T) D^-_{\mathbf{K}_f}(\mathbf{R}) | W_i | \Phi^+_i(\mathbf{r}_T, \mathbf{R}_T) > \qquad (4)$$

and from this the six dimensional cross section is thereafter obtained in the standard way:

$$\frac{d\sigma}{dE_T \, dE_{K_f} \, d\Omega_{\mathbf{k}_T} \, d\Omega_{\mathbf{K}_f}} = k_T K_f \frac{(2\pi)^4}{v} |T_{fi}|^2 \qquad (5)$$

Here $E_T = 1/2k_T^2$ is the final electronic energy and $E_{K_f} = 1/(2\mu)K_f^2$ the energy associated with the heavy particles in the final channel.

When only interested in the double differential cross section for the ejected electron, we have to integrate the $\mathbf{K}_f$-coordinate out of the expression in eq. 5 :

$$\frac{d\sigma}{dE_T \, d\Omega_{\mathbf{k}_T}} = \frac{k_T (2\pi)^4}{v^2} \int d\mathbf{K}_f |T_{fi}|^2 \delta(\hat{\mathbf{v}}\mathbf{K}_f - K_i + \frac{1/2k_T^2 - \epsilon_i}{v}). \qquad (6)$$

The last energy-conservation delta-function guaranties that only processes which are allowed by energy conservation are summed. We are accordingly left with a two-dimensional integration over the components of $\mathbf{K}_f$ perpendicular to $\mathbf{v}$.

Using Parsevel's theorem we may transform eq. 6 to a two dimensional integration of the Fourier transform of the T-matrix. Defining $\mathbf{K}_{f\parallel}$ and $\mathbf{K}_{f\perp}$ as the components of $\mathbf{K}_f$ parallel and perpendicular to $\mathbf{v}$ respectively, the two dimensional Fourier transform of the T-matrix in eq. 4 is given by

$$\tilde{T}_{fi} = (2\pi)^{-1/2} < \psi_{\mathbf{k}_T}(\mathbf{r}_T, \mathbf{R}_T) \exp(i\mathbf{K}_{f\parallel}\mathbf{R}_T) D^-_f(\mathbf{R}_T) \times$$
$$\{\tfrac{1}{(2\pi)^2} \int d\mathbf{K}_{f\perp} \exp(i(\mathbf{R}_T - \mathbf{b})\mathbf{K}_{f\perp})\} | W_i | \Phi^+_i(\mathbf{r}_T, \mathbf{R}_T) > \qquad (7)$$

where we have neglected the explicit dependence on $\mathbf{K}_{f\perp}$ in $D^-_{\mathbf{K}_f}$ (this approximation is equivalent to a straight line Eikonal approximation which is commonly accepted as an accurate approximation in ion-atom collisions).

In order to proceed we need to write the initial wave function in a form similar to the final wave function in eq. 3,

$$\Phi^+_i(\mathbf{r}_T, \mathbf{R}_T) = \varphi_T \varphi_{\mathbf{K}_i}(\mathbf{R}_T) D^+_{\mathbf{K}_i}(\mathbf{R}_T). \qquad (8)$$

Here $D^+_{\mathbf{K}_i}(\mathbf{R}_T)$ is a distortion factor describing the elastic scattering of the heavy particles due to the distortion potential U_i. The inner integral over $\mathbf{K}_{f_\perp}$ in eq. 7 gives a delta function, which takes away two dimensions from the outer integral. We finally find

$$\tilde{T}_{fi} = (2\pi)^{-2} \int_{-\infty}^{\infty} dZ \ \exp(i(K_i - K_{f_\parallel})Z)[D^-_f(\mathbf{R}_T)]^* D^-_{\mathbf{K}_i}(\mathbf{R}_T) \times (\psi_{\mathbf{k}_T}(\mathbf{r}_T, \mathbf{R}_T)|W_i|\varphi_T(\mathbf{r}_T, \mathbf{R}_T))_{\mathbf{r}_T} \quad (9)$$

where the inner integral, $(\ |\ |\ )_{\mathbf{r}_T}$, is a three dimensional integral over $\mathbf{r}_T$.

3 Determining distortion potential and perturbation in the initial channel

When the T–matrix is examined in a multichannel representation it appears natural to choose the distortion potential in such a way that diagonal terms in the coupling matrix vanishes [9]:

$$< \Phi_i^+|E - H|\Phi_i^+ >= 0 \quad (10)$$

The perturbation W_i will depend on how we choose the heavy particle distortion potential and which potentials are included in the electronic part of the functions, φ_T. For slow projectile velocities it is natural (and essential) to choose a molecular or two-center wave function for φ_T. For fast and intermediate velocities we may approximate φ_T by an atomic state.

At first we define a distortion potential and a perturbation operator in the molecular picture. In this case φ_T is the solution of the equation

$$h\varphi_T(\mathbf{r}_T, R_T) = \epsilon_i(R_T)\varphi_T(\mathbf{r}_T, R_T) \quad (11)$$

where

$$h = -\frac{1}{2}\nabla^2_{\mathbf{r}_T} + V_T(r_T) + V_P(r_P). \quad (12)$$

is the electronic two-center hamiltonian and is $\epsilon_i(R_T)$ is the electronic (adiabatic) term. Both φ_T and ϵ_i depends parametrically on the distance, R_T, between the heavy particles.

Substitution of eq. 8 with φ_T defined by eq. 11 into eq. 10 we obtain in the eikonal approximation a distortion factor $D^+_{K_i}$, of the following form:

$$D^+_{K_i}(\mathbf{R}_T) = \exp\{-\tfrac{i}{v}\int^Z U_i(\mathbf{b},\tilde{Z})\,d\tilde{Z}\},$$
$$U_i(\mathbf{R}) = -\epsilon_T + \epsilon_i(R) + V_{PT} + \tfrac{1}{2\mu}H_{ii}(R) \qquad (13)$$

where ϵ_T is the electronic binding energy and the diagonal non-adiabatic matrix element H_{ii} is given by

$$H_{ii} = (\varphi_T|\nabla^2_{\mathbf{R}_T}|\varphi_T). \qquad (14)$$

Using this initial state we from eq. 2 obtain the perturbation

$$W_i = iv\frac{\nabla_{\mathbf{R}_T}\varphi}{\varphi} + \frac{1}{2\mu}\{\frac{\nabla^2_{\mathbf{R}_T}\varphi}{\varphi} - H_{ii}\} \qquad (15)$$

Secondly, using an atomic state as φ_T we may similarly derive the following distortion potential and perturbation:

$$U_i = (\varphi_T|V_P|\varphi_T)_{\mathbf{r}_T} + V_{PT}$$
$$W_i = V_P - (\varphi_T|V_P|\varphi_T)_{\mathbf{r}_T} \qquad (16)$$

The distortion potential for the heavy particles in the final channel could in principal be derived in a similar way. To order $O(\frac{1}{\mu})$ we find:

$$U_f(R) = V_{PT}(R) \qquad (17)$$

This approximation of the final distortion potential is equivalent to neglecting the continuum-continuum coupling [4,5].

Going back to eq. 9, our final expression for the Fourier transform of the T-matrix is therefore given by:

$$\tilde{T}_{fi} = (2\pi)^{-2}\int_{-\infty}^{\infty} dZ\ \exp(-\tfrac{i}{v}S(\mathbf{b},Z))$$
$$(\psi_{\mathbf{k}_T}(\mathbf{r}_T,\mathbf{R}_T)|W_i|\varphi_T(\mathbf{r}_T,\mathbf{R}_T))_{\mathbf{r}_T} \qquad (18)$$

where $S(\mathbf{R})$ is given by

$$S(\mathbf{b},Z) = \int^Z \{U_i(\tilde{z},\mathbf{b}) - U_f(\tilde{z},\mathbf{b}) + \epsilon_T - E_T\}\,d\tilde{z}). \qquad (19)$$

Here we have used the energy conservation condition $K_{f_\parallel} - K_i = (\epsilon_T - E_T)/v$.

4 The T-matrix in the stationary phase approximation

For small collision velocities, ($v \ll 1$), $\frac{1}{v}S(\mathbf{b}, Z)$ in eq. 18 is large and therefore the phase oscillates rapidly. In this case the main contribution to the Z-integration is drawn in the vicinity of the stationary phase points. The stationary points (or saddle points) are determined by the equation:

$$\frac{d}{dZ}S(\mathbf{b}, Z) = 0 \tag{20}$$

which corresponds to the points, Z_*, satisfying

$$U_i(\mathbf{b}, Z_*) + \epsilon_T = U_f(\mathbf{b}, Z_*) + E_T \tag{21}$$

Evaluating the integral in eq. 18 in the stationary point approximation we obtain

$$T_{fi} = \frac{1}{(i\hbar)^2} \sum_{Z_*=\pm} \sqrt{|d/dz(U_i - U_f)|} \exp\{-\frac{i}{v}S(\mathbf{b}, Z) + \frac{i\pi}{4}Sign(d/dz(U_i - U_f))\}$$
$$\langle \psi_{\mathbf{k}_T}(\mathbf{r}_T, \mathbf{R}_*)|W_i|\varphi_T(\mathbf{r}_T, \mathbf{R}_*)\rangle|_{Z=Z_*} \tag{22}$$

At threshold, ($k_T = 0$), we introduce the difference

$$w(\mathbf{b}, Z) = U_i(\mathbf{b}, Z) + \epsilon_T - U_f(\mathbf{b}, Z) \tag{23}$$

In collisions between negative heavy particles, M^- (μ^-, π^-, K^- and $\bar{p}$), and atomic systems, A, it is readily shown that eq. 23 has roots on the real axis, $R_T(b, Z) = R_S$, and that for $R_T \leq R_S$

$$w(R_T) \geq 0 \tag{24}$$

This indicates that for $R_T \leq R_S$ the quasi-molecular system, (M^-A), can make classically allowed transitions which leads to ionization). A typical view of the potentials is shown in figure ... The energy of the ejected electron is determined by the transition ... $= w(R_T)$ (see figure 1.). In the region $R_T \leq$ ... cluster ... be interpreted as a "quasi-molecule" in an ... n s... total width of decay given by

$$\Gamma(R) = \pi \qquad E_T - w(R_T).$$

We can utilize the total decay width to determine an intuitive normalization

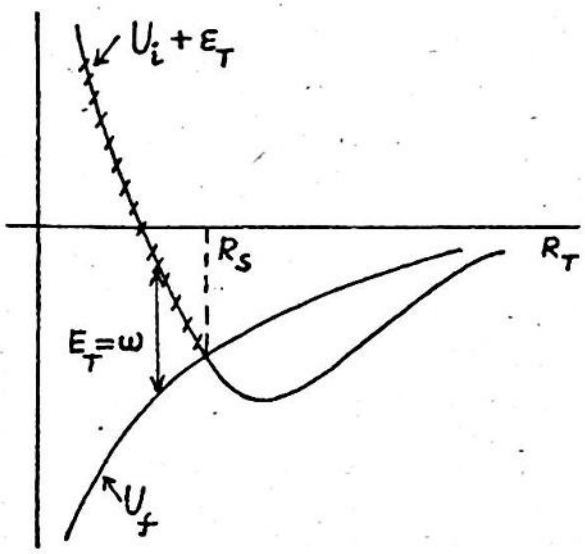

Fig 1: Distortion potentials in the initial and final channels. The intersection point, R_s corresponds to the boundary of the continuum for $(M^- A) \to M^- + A^+ + e$, $(E_T = 0)$. The dashed part of the U_i-curve indicates that for $R < R_s$ the system $(M^- A)$ may decay classically.

of the autoionization state [8]. However, when the amplitude for finding the electron in a particular state decreases, the amplitude for finding the heavy particle system in the initial channel decreases in a similar way. We may accordingly write a normalization for the heavy particle wave function as:

$$\varphi_{K_i}(\mathbf{R}_T) D^+_{K_i}(\mathbf{R}_T) \to \exp(-\frac{1}{2}\int^{R_T} \frac{\Gamma(\mathrm{b}, \tilde{Z})}{v}\, d\tilde{Z}) \varphi_{K_i}(\mathbf{R}_T) D^+_{K_i}(\mathbf{R}_T) \quad (26)$$

We finally obtain the expression for the double differential cross section as

$$\frac{d\sigma}{dE_T\, d\Omega_{k_T}} = \frac{k_T}{v} \sum_{Z=Z_s} \int d\mathrm{b}\, \frac{\Gamma_{k_T}(\mathrm{b}, Z_s) P(\mathrm{b}, Z_s)}{|d/dZ(U_i - U_f)|} \quad (27)$$

where

$$\Gamma_{k_T} = 2\pi |(\psi_{k_T}|W_i|\varphi_T)|^2|_{E_T = \omega(R_S)} \quad (28)$$

is the partial width of decay at point $\mathbf{R}_T = \mathbf{R}_s$ and

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$$\Gamma(R) = 2\pi \int dE_T\, d\hat{\mathbf{k}}\, |(\psi_{\mathbf{k}}|W_i|\varphi_T)|^2\delta(E_T - w(\mathbf{R}_T). \tag{25}$$

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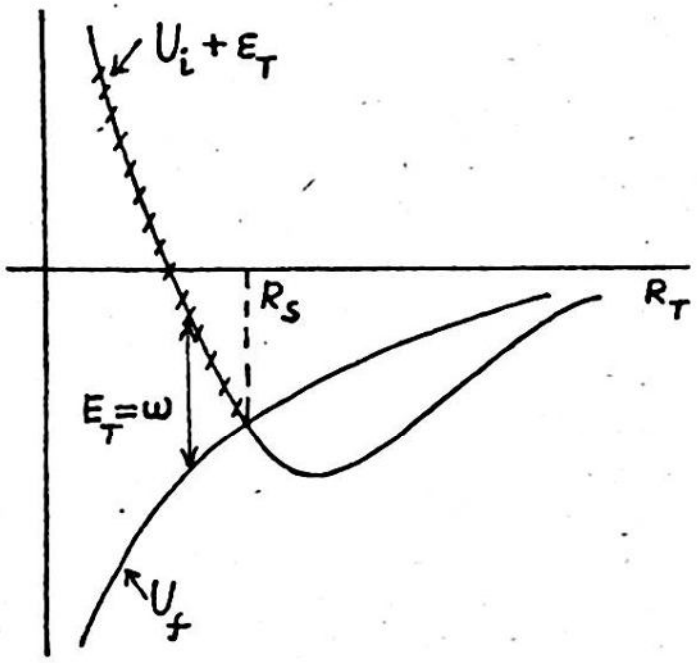

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vanishing contribution due to the rapid oscillations and has been neglected in eq. 27.

5 Conclusion

We have derived a theory for low and intermediate energy collisions between heavy negative particles and simple atoms. This theory may be extended to slow positive projectile impact if the stationary phase approximation is replaced by a saddle point approximation in the complex plane. As is always the case in scattering physics, the quality of the final result depends on how accurate the initial and final wave functions are represented. It was therefore shown how to employ both an atomic as well as a molecular descriptions of the electronic state. The expression for the transition amplitude emerged in an intuitive and simple form which allows a clear physical understanding of the scattering process. Our result is accordingly interesting form a purely theoretical approach as well as form a computational approach, since cross sections may be obtained by a simple three dimensional integration in the low and intermediate energy limit.

6 Acknowledgments

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Товчлол

Сөрөг цэнэгтэй удаан бөөмс, атомтай мөргөлдөх үзэгдлийг илэрхийлэх аргыг Т-матрицын дөхөлтөнд боловсруулсан.

Хүнд бөөмсийн харьцангуй хөдөлгөөнд эйкональ ойролцоолол хэрэглэж Т-матрицын ерөнхий илэрхийллийг стационар фазын ойролцоололд гарган авлаа.

Иончлолллын огтлол нь нэг талаас мөргөлдөөний үед үүссэн квазимолекуляр систем задрах өргөн, нөгөө талаас удаан бөөм харимхай сувагтаа үлдэх магадлал хоёрын үржвэр хэлбэртэй бичигдэхийг үзүүлсэн болно.

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