Influence of Post-Collision-Interaction in Auto-ionization

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Abstract. Following the ideas of Senashenko [8] we obtain an expression for the resonant part of the auto-ionizing transition matrix consisting of the standard first Born expression, and an additional factor containing the remaining effects of Post-Collision-Interaction. This factor becomes very important when one studies the angular dependence of auto-ionization from spherical symmetric auto-ionization states. We in particular concentrate on decay form the $(2s^2)^1S$ state since an experimental investigation of this process has recently been published [2]

1. Introduction

The electron emission by particle impact on effective two–electron target systems is normally understood to evolve along two separate path: One path - the direct transition - is a fast *knock out* process where the electron is kicked into the continuum, while the other path is a much slower process, where the projectile excites long lived auto-ionization states in the two-electron target system, and continues on its trajectory for a very long time before the auto-ionizing state decays, leaving one electron in a bound state and one in the continuum. The transition amplitude is therefore split into two parts: one describing the direct transition form the asymptotic initial state to the final state and one describing the transition via intermediate states. The reasons for this separation are both practical and theoretical: Due to physical insight into the scattering process, we may use different approximations in the calculation of T_{Dir} and T_{Res} respectively, and theoretically the separation of the transition amplitude allows a physical interpretation of the ionization process. The interaction between the projectile and the excited target auto-ionizing state, at the time of decay, as well as the projectile–electron interaction after decay has normally been neglected due to the spacial separation of the projectile and the target system at this time. However, the long range nature of the Coulomb interaction may over very long distances influence both the decay process as well as the trajectory of the electron after decay. This Post-Collision-Interaction (PCI) has been studied by Senashenko [8] as well as number of other authors (see ex. [5] [1] [7]). Recently Balashov *et al* [2] experimentally extracted the angular dependence of the *resonant* part of the transition amplitude from previous measurements of the Shore a, b and f parameters [9]. Even though quite different results were obtained when utilizing the Shore parameters measured by different groups, a strong effect on the resonant part

of the transition matrix was observed from *spherical symmetric* $(2s^2)^1S$ states. Since this angular dependence can not result from a first Born treatment, it appears to be a clear indication of PCI. We will in the following show that such an interaction is in fact present but further investigations are necessary to reproduce the experimental data.

The notation will follow the one used by Senashenko [8]: The projectile, target nucleus, and the two electrons are numbered from one to four respectively, while the vector pointing from particle i to particle j is denoted $\mathbf{r}_{ij}$ (as usual we will however, write the vector pointing from the target to the projectile as R). The charge of the projectile and the target nucleus are Z_P and Z_T respectively, and the Sommerfiet parameter referring to the relative motion of particle i and j is given by $\nu_{ij} = Z_i Z_j m_{ij}/k_{ij}$, where m_{ij} and k_{ij} is the reduced mass and the relative momentum of particle i and j. Plane waves will be written as $\phi_k(\mathbf{r}) = (2\pi)^{-3/2}\exp(i\mathbf{kr})$ and Coulomb waves in the field of the charge Z, by $\psi_k^{Z+}(\mathbf{r})$. Atomic units are used throughout unless otherwise noticed.

2. THE DERIVATION OF THE T-MATRIX

From the standard T-matrix in the prior form, we readily obtain a form suitable for a separation of the T-matrix in a direct and a resonance part:

$$T_{if} = < \psi_f|H - E|\Phi_i > + < \Psi_f^- - \psi_f|H - E|\Phi_i > = T_{Dir} + T_{Res} \qquad (1)$$

where the asymptotic state in the final channel, ψ_f, (possible including some long–range Coulomb interactions) have been separated from Ψ_f^-, to allow a separation of the direct, T_{Dir}, and the resonant, T_{Res}, part of the transition amplitude. We will limit our self to the case where one electron ends up in the continuum while the other falls into a 1s hydrogenic state on the target ion. Since the size of this bound state is small, we will approximate the final state wave–function as a product state factorized by a 1s hydrogenic wave–function, $\varphi_f(r_{24})$, and a part describing an electron in the continuum of two charges. For this last part we employ the continuum 3–center wave function first suggested by Remond and later use by a number of authors (see ex. [3]). Explicitly, we write the final channel wave–function as

$$\begin{aligned}\Psi^- = {} & N^*(\nu_{13})N^*(\nu_{21})\,{}_1F_1(i\nu_{21},1,-i(k_{21}R + \mathbf{k}_{21}\mathbf{R})) \times \\ & {}_1F_1(i\nu_{13},1,-i(k_{13}r_{13} + \mathbf{k}_{13}\mathbf{r}_{13}))\psi_{k_{23}}^{Z_T-}(\mathbf{r}_{23})\phi_{K_{12}}(\mathbf{R}_{12})\varphi_{1s}(r_{24}) \qquad (2)\end{aligned}$$

where $N(\nu)$ is the Coulomb normalization constant.

To project out the intermediate auto-ionization states from the total wave function we define the following projection operators:

$$\begin{aligned} Q &= \sum_{i\subset\Omega} |\varphi_i(\mathbf{r}_1,\mathbf{r}_2) >< \varphi_i(\mathbf{r}_1,\mathbf{r}_2)| \\ P &= \sum \int_{i\subset\Omega^c} |\tilde{\varphi}_i(\mathbf{r}_1,\mathbf{r}_2) >< \tilde{\varphi}_i(\mathbf{r}_1,\mathbf{r}_2)|. \end{aligned} \qquad (3)$$

Here Ω is the subset of the entire two-electronic Hilbert space, which contains the auto-ionizing states (in the following denoted by $\varphi_i(\mathbf{r}_1, \mathbf{r}_2)$), while Ω^C is everything else. Notice however, that the Q and P operators are only acting on the electronic coordinates. We accordingly *within the two-electronic Hilbert space* have

$$P + Q = 1 \qquad PQ = QP = 0 \qquad P^2 = P \qquad Q^2 = Q \tag{4}$$

The Schrödinger equation may now be written

$$< \Psi_f^- | (H - E^-) = (< \Psi_f^- P^* | P + < \Psi_f^- Q^* | Q)(H - E^-) = 0 \Rightarrow$$
$$< \Psi_f^- P^* | P(E^- - H)P = < \Psi_f^- Q^* | QHP \quad < \Psi_f^- Q^* | Q(E^- - H)Q = < \Psi_f^- P^* | PHQ \tag{5}$$

We now proceed to define a Greens operator and subsequently write a formal expression for $< \Psi_f^- P^* | = < \psi_f | P + < \Psi_f^- Q^* | QHPG_P^-$. Here $< \psi_f |$ is the solution to the homogeneous equation (physically corresponding to the asymptotic state) and, $G_P^- = [P(E - i\eta - H)P]^{-1}$, is the Greens operator. Substituting this expression into the second equation in eq. 5 we find

$$< \Psi_f^- Q^* | Q(E^- - H - HPG_P^- PH)Q = < \psi_f | PHQ \Rightarrow$$
$$< \Psi_f^- Q^* | = < \psi_f | PHQG_Q^- \tag{6}$$

where the Greens operator G_Q^- is given by

$$G_Q^- = [Q(E - i\eta - H - HPG_P^- PH)Q]^{-1} \tag{7}$$

Finally using the expression in eq. 6 in the expression for $< \Psi_f^- P^* |$ we find

$$< \Psi_f^- P^* | = < \psi_f | P + < \psi_f | PHQG_Q^- QHPG_P^- \tag{8}$$

The total wave function corresponding to the asymptotic final channel, $< \psi_f |$, is now given by

$$< \Psi_f^- | = < \Psi_f^- P^* | + < \Psi_f^- Q^* | = < \psi_f | P + < \psi_f | PHQG_Q^- (1 + QHPG_P^-) \tag{9}$$

The corresponding T-matrix is accordingly

$$T_{fi}^- = T_{Dir}^- + T_{Res}^- = < \psi_f | (H - E) | \Phi_i > +$$
$$< \psi_f | PHQG_Q^+ (1 + QHPG_P^+)(H - E) | \Phi_i > \tag{10}$$

where $|\Phi_i>$ is the initial wave function. The Greens functions are derived by Senashenko [8] and the final expression for the resonant part of the transition matrix, it its prior form, is given by

$$T_{Res}^- = \sum_\mu \tau_{exc} \tau_{dec}^0 K_{res,\mu} \tag{11}$$

e τ_{ex} is the excitation amplitude from the initial electronic state to the auto-ing state and τ^0_{dec} is a decay amplitude from the auto-ionizing state to the one-r Coulomb state

$$\tau^0_{dec} = < \varphi_{1s}(r_{24}) \psi^{Z_T -}_{k_{23}}(\mathbf{r}_{23}) | V | \Phi_\mu > \qquad (12)$$

PCI-effects are embedded in the $K_{res,\mu}$ factor given by

$$_{res,\mu} = -(E_e - E_\mu + i\Gamma_\mu/2) N(\nu_{13}) N(\nu_{21}) \frac{2\mu_a}{4\pi} \int d\mathbf{R} \, \frac{\exp(iK_r R)}{R} \times$$
$$_1F_1(-i\nu_{21}, 1, i(k_{21}R + \mathbf{k}_{21}\mathbf{R}))\, _1F_1(-i\nu_{31}, 1, i(k_{31}R - \mathbf{k}_{31}\mathbf{R})). \qquad (13)$$

$K_r = [k^2_{21} + (2\mu_a(E_e - E_\mu + i\Gamma_\mu/2)]^{1/2}$ (E_e and E_μ being the energies of the ed electron and the auto-ionizing state respectively). Two approximations were loyed to derive the result in eq. 11. First of all we only included the transi-s from the asymptotic state to the final state via *one* intermediate auto-ionizing e (we accordingly neglected the transition between different auto-ionizing states), secondly we approximated the interaction between the projectile and the target em *not embedded in the final three-center wave function* by the static potential esponding to the different auto-ionizing states

$$\frac{Z_P}{|\mathbf{R} - \mathbf{r}_{23}|} + \frac{Z_P}{|\mathbf{R} - \mathbf{r}_{24}|} \rightarrow < \varphi_\mu(\mathbf{r}_1, \mathbf{r}_2) | \frac{Z_P}{|\mathbf{R} - \mathbf{r}_{23}|} + \frac{Z_P}{|\mathbf{R} - \mathbf{r}_{24}|} | \varphi_\mu(\mathbf{r}_1, \mathbf{r}_2) > \qquad (14)$$

se are both standard approximations, the last one corresponding physically to the umption that the projectile-impact excitation and the decay of the auto-ionization e is separated in time due to the comparative long lifetime of the double excited e.

3. DISCUSSION

physical understanding of auto-ionization is *not a two step process but a three process*. First the target atom is excited into the auto-ionizing state, secondly the o-ionizing state decays leaving one electron in the continuum and one in a bound e, and thirdly the ionized electron moves towards the detector. Due to the long time of the auto-ionizing state the projectile moves far enough away to neglect the jectile Coulomb interaction on the decay of the *neutral target system*. However oon as the electron is in the continuum it is no longer shielded by being part neutral target system and is subject to both the interaction from the projectile well as from the residual target ion. The approximation employed in this paper ct this understanding of the scattering process: we included the effect of PCI on the final electronic state. The inclusion of the $K_{res,\mu}$-factor in 11 is a result he three step model, and reflects the effect of PCI.

When auto-ionization is understood as a pure two-step process (combining the last phases described above) the electron-projectile interaction is neglected while emitted electron is in the continuum. In this case, the exited target-state as

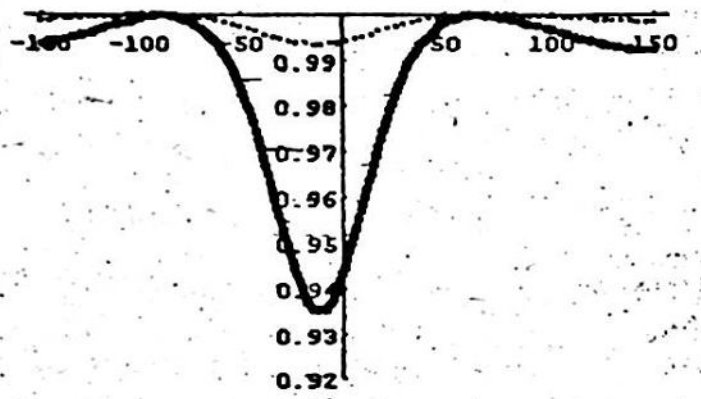

Figure 1: The modules of the K-factor as a function of electron emission angle (deg). The thick and dotted curves correspond to a projectile energies of 200 eV and 400 eV, respectively (see the text for more details).

well as the final electronic continuum state does not depend on the direction of the projectile neither before nor after the excitation. The resonant part of the T–matrix, T_{Res}, accordingly only depends on the auto–ionizing state for its angular dependence. This is especially interesting in the case of *spherical symmetrical S-state resonances*. In this case the angular dependence of T_{Res} vanishes when the PCI is neglected. When measuring S–state resonances, any angular dependence in T_{Res} is accordingly a clear indication of the importance of PCI. Balashov *et al* [2] derived a way to obtain T_{Res} from measurements of the Shore parameters. They explicitly extracted a c–parameter, given by $c = T_{Res}(\epsilon_r + i)$. Comparing with the expression in eq. 11 it becomes clear that the angular dependence found in |c| for auto-ionization from doubly excited S-states is embedded in the K_{res}–factor. This Nordsick integral (13) is easily derived analytically (see ex. [10]), and we find

$$K_{res,\mu} = -((E_e - E_\mu + i\Gamma_\mu/2)N(\nu_{13})N(\nu_{21})2\mu_a \frac{C^{-i\nu_{21}-i\nu_{31}-1}}{A^{-i\nu_{21}}B^{-i\nu_{31}}} {}_2F_1(-i\nu_{31}, -i\nu_{21}, 1, Z) \quad (15)$$

where

$$A = (K_r + ik_{21})^2 \quad B = (K_r + ik_{31})^2 + (k_{31} + k_{21})^2 \quad C = K_r^2 - k_{21}^2$$
$$Z = 2\frac{A(k_{31}k_{21} - ik_{31}K_r) + C(ik_{31}K_r + k_{21}k_{31})}{AB} \quad (16)$$

In figure 1 we show the calculation of the modules of the K_{res}–factor as a function of the electron ejection angle, θ_{ej}, for the $(2s^2)^1S$ auto-ionizing state in He, excited by electron impact at $E_0 = 200\,eV$ at scattering electron angle $\theta_{sc} = -12°$. Even though the variation is smaller than the one reported in the Balashov paper, it appears that the general behavior of $|K_{res}|$ corresponds to the behavior of $|c|$ as a function of θ_{ej}. In figure 2 we show the phase dependence of the K_{res}–factor under similar conditions

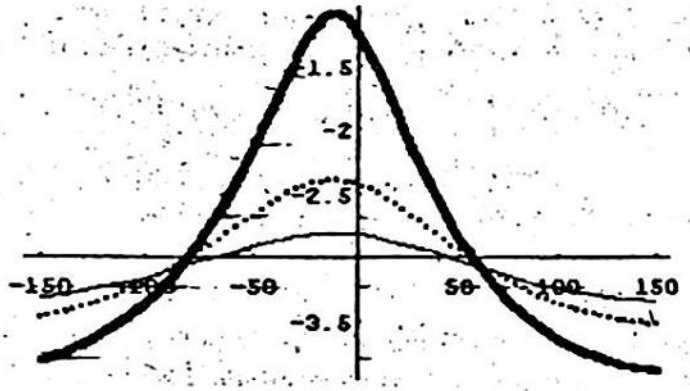

Figure 2: The phase (in rad.) of the K-factor as a function of electron emission angle (deg). The thick, dotted and line curves correspond to projectile energies E=200eV, E=400eV and E=800eV respectively (see text for more details).

as in figure 1. Here the variation is much more obvious. The effects of Coulomb perturbations normally appear strongest in the phases of the transition amplitudes. It follows that the expression in eq. 11 to a good approximation for a single resonance may be written as

$$T^{-}_{Res,\mu} = \tau_{ex}\tau^{0}_{dec}\exp(i\Phi(\mu,\theta_{ej})) \qquad (17)$$

where PCI effects are contained in $\exp(i\Phi(\mu,\theta_{ej}))$. However, as show in figure 2, the effects of PCI decreases as the collision energy increases. This is expected since the standard approximations, which neglect PCI ($\exp(i\Phi(\mu,\theta_{ej})) \approx 1$), are valid for high energy collisions. Sometimes, as in the case of Coulomb scattering in a one-center fields, this phase is hidden experimentally since only the modules of the transition amplitude is important (see ex. [4]). At other times the a Coulomb perturbation from a third particle can lifts an approximated two-body scattering process *off the two-body energy-shell*, and the perturbation again shows up in an extra Rutherford phase factor. This is the case in ionization from fast ion-atom collisions [6]. To our knowledge eq. 17 is the first time this Coulomb perturbation phase factor is observed in T_{Res}. Here however, it is much more important than in the other two cases, due to the interference with the direct part of the transition amplitude.

As shown above, the inclusion of the PCI–effects partly breaks down the standard pure two-step description of auto-ionization. The strong phase dependence of the K_{res}–factor, shown in figure 2, will give rise to interference with the direct part of the scattering amplitude. This interference will in turn result in effects poorly represented by the Shore parameters. Since the Shore parameters and subsequently the definition of the c–parameter are defined on the unrealistic assumption that PCI can be neglected, the measurement reported by Balashov may have to be reinterpreted.

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