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A comment on the Influence of Post-Collision-Interaction and experimental resolution in Auto-ionization

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Abstract

Following the ideas of Balashow, Martin and Crowe [1] we have isolated the resonant part of the transition amplitude for auto-ionization from the $(2S^2)^1$ state, in several different ways: 1.) from the pure theoretical T-matrix, 2.) from the theoretical cross section using Shore parameters [2] and 3.) from an "experimental" cross section where the theoretical cross section has been convoluted with an experimental resolution. Our conclusion is that the variations of the o-parameter reported in [1] is a result of both post-collisional interaction as well as an effect of the experimental resolution.

1 Introduction

Electron emission by particle impact on effective two–electron target systems is normally understood to evolve along two separate routes: One - the direct transition - is a fast *knock out* process where the electron is kicked into the continuum, while the other route 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 accordingly split into two parts: one describing the direct transition, T_{Dir}, form the asymptotic initial state to the final state and one, T_{Res} describing the transition via intermediate auto-ionizing 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 and ionized-electron interaction after decay, have 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 long distances influence both the decay process as well as the trajectory of the ionized electron after decay. This Post-Collision-Interaction (PCI) has been studied by Senashenko [3] as well as number of other authors.

Recently Balashow *et al* [1] extracted the angular dependence of the *resonant* part of the transition amplitude from previous measurements of the a, b and f Shore parameters [2]. 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 and seems to be magnified by experimental resolution.

The notation will follow the one used by Senashenko [3]: 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 $\mathbf{R}$). The charge of the projectile and the target nucleus are Z_P and Z_T respectively, and the Sommerflet 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

$\phi_{\mathbf{k}}(\mathbf{r}) = (2\pi)^{-3/2}\exp(i\mathbf{kr})$ and Coulomb scattering states in the field of the charge Z, by $\psi_{\mathbf{k}}^{Z+}(\mathbf{r})$. 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:

$$T_{fi} = <\psi_f|H-E|\Phi_i> + <\Psi_f^- - \psi_f|H-E|\Phi_i> = T_{Dir} + T_{Res} \tag{1}$$

where the asymptotic state in the final channel, ψ_f, have been separated from Ψ_f^-, to allow an isolation 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 residual target ion. Since the size of this bound state is small, the final state is written as a product of 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 Redmond and later use by a number of authors (see ex. [5]). Explicitly, we write the final channel wave–function as

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

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

Inserting eq. 2 in eq. 1 we obtain the following expressions for T_{Dir} and T_{Res}:

$$T_{fi} = <\Psi^-|V_i|\varphi_{He}(r_{23},r_{24})\phi_{\mathbf{K}_i}(\mathbf{R})> + K^{\mu}_{Res} <\psi_{\mathbf{k}_{23}}^{Z_T-}(\mathbf{r}_{23})\phi_{\mathbf{K}_{21}}(\mathbf{R})\varphi_{1s}(r_{24})|V_i|\varphi_{He}(r_{23},r_{24})\phi_{\mathbf{K}_i}(\mathbf{R})> \tag{3}$$

where the perturbation, V_i, is the projectile–target atom interaction, and φ_{He} is the helium wave function. In this calculation we will approximate this by the product of two 1s hydrogenic states with an effective central charge $Z_{eff} = 1.6875$ (see ex. Landau and Lifshitz, Quantum Mechanics). The resonant part of the T-matrix in eq. 3 was derived by Senashenko [3], who derived the K-factor

$$\begin{aligned}K_{res,\mu} = {} & -(E_e - E_\mu + i\Gamma_\mu/2)N(\nu_{13})N(\nu_{21})\frac{2m_{12}}{4\pi}\int d\mathbf{R}\,\frac{\exp(i(\mathbf{K}_r\mathbf{R}-\mathbf{k}_{21}\mathbf{R}))}{\mathbf{R}}\times \\ & {}_1F_1(-i\nu_{21},1,i(k_{21}R+\mathbf{k}_{21}\mathbf{R}))\,{}_1F_1(-i\nu_{31},1,i(\mathbf{k}_{31}\mathbf{R}-\mathbf{k}_{31}\mathbf{R})).\end{aligned} \tag{4}$$

where Γ_μ is the width of the auto-ionizing state and $K_r = [k_{21}^2 + (2m_{12}(E_e - E_\mu + i\Gamma_\mu/2)]^{1/2}$ (E_e and E_μ being the energies of the ejected electron and the auto–ionizing state respectively). The direct part of the transition amplitude in eq. 3 is similar to the one used by Brauner, Briggs and Broad [4] to derive the direct triply differential cross section for ionization of helium by electron impact.

Experimental measurements of auto-ionizing resonances has traditionally been parameterize using Shore parameter [2] in the following way:

$$\frac{\sigma^3}{d\Omega_{k_{23}}\,d\Omega_{k_{21}}\,dE_e} = f(\mathbf{k}_{21}^f,\mathbf{k}_{23}) + \frac{a(\mathbf{k}_{21}^f,\mathbf{k}_{23})\epsilon_r + b(\mathbf{k}_{21}^f,\mathbf{k}_{23})}{\epsilon_r^2+1} \tag{5}$$

where ϵ_r is the deviation of the excitation energy from the resonance measured in terms of its half-width:

$$\epsilon_r = \frac{E_e - E_\mu}{\Gamma_\mu/2} \tag{6}$$

and $f(\mathbf{k}_{21}^f,\mathbf{k}_{23})$ is proportional to the norm square of the direct part of the transition amplitude.

Fano [6] derived his famous expression for the resonance part of the transition amplitude as:

$$T_{Res} = t_{dir}^l\frac{q_r - i}{\epsilon_r + 1} \tag{7}$$

where q_r is the profile function (see. Jacob) and t^l_{dir} is the first Born direct amplitude for the partial wave l. Using this form Balashow *et al* [1] wrote the cross section as

$$\frac{\sigma^3}{d\Omega_{k_{23}}\, d\Omega_{k_{21}}\, dE_e} = (2\pi)^4 \frac{k_{23}}{k_{21}} ||T_{Dir}|e^{i\beta} + \frac{|c|}{\epsilon_r + i}|^2 \qquad (8)$$

where $\beta = argT_{Dir} - argc$ and $c = t^l_{dir}(q_r - i)$. Combining eq. 5 and eq. 8 they obtained an second order equation for the modulus of the c-parameter. Solving this equation we find that $|c|^2$ may be written terms of the Shore parameters, a, b and f as

$$|c^{\pm}|^2 = b + 2f \pm \sqrt{4f^2 + 4bf - a^2} \qquad (9)$$

3 The effect of Post-collisional interaction on $|c|^2$

Studying the $(2s^2)^1S$ resonance in Helium in the way described above, it is expected that the modulus of the c-parameter should be independent on the ejection electron ejection angle, since $t^{l=0}_{dir}$ in eq. 7 is angular independent due to the spherical symmetry of the auto-ionization state. However, when inserting experimental measurement of the a, b and f in eq. 9, Balashow *et al* found a strong dependence on the ejection angle.

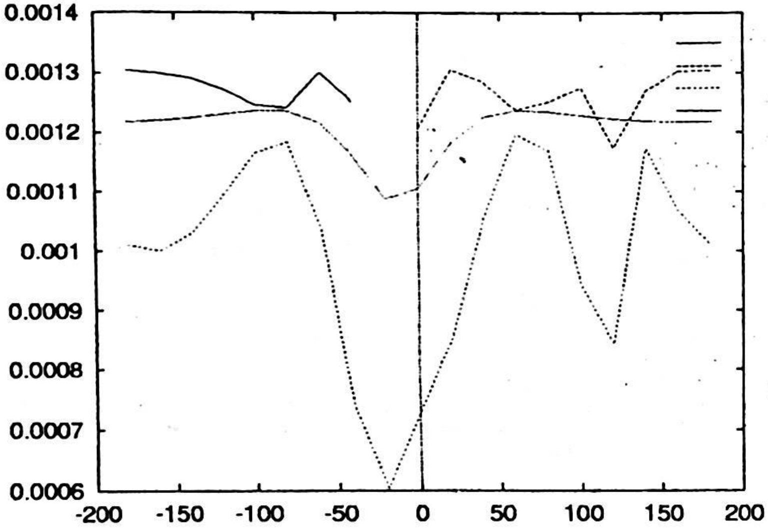

Figure 1: $|c|^2$ calculated for 200 eV. electron impact on Helium, for the $(2S^2)^1$ resonance, with a scattering angle $\theta_{sca} = -13°$, as a function of electron ejection angle. The solid curve and the upper dotted curve correspond to $|c|^2$ derived from the theoretical cross sections. In between the two curves, in the region around $\theta = -13°$, the fitting with Shore parameters resulted in a complex $|c|^2$. The dashed curve is the theoretical $|c|^2$ and the lower dotted curve corresponds to $|c|^2$ obtained from theoretical cross sections convoluted with an experimental resolution of 150 meV.

Including some post-collisional interaction in the way describe in section 2 we may from eq. 3 and 8 isolate $|c|^2$ from

$$|c| = |(\epsilon_r + i)K^{\mu}_{Res} < \psi^{Z_T -}_{k_{23}}(r_{23})\phi_{K_{21}}(R)\varphi_{1s}(r_{24})|V_i|\varphi_{He}(r_{23}, r_{24})\phi_{K_i}(R) > \qquad (10)$$

Even though this do give rise to some angular dependence of —c—, it does not seem to be enough to describe the strong variation observed by Balashow *et al*, see the figure. To check the quality of the Shore parameterization on the spectrum when PCI was included in the calculation, we fitted the cross section derived from eq. 3 with the Shore parameters (eq. 5), and in turn obtained $|c|^2$ from eq. 9. When the ionized electron is ejected parallel to the projectile, the post-collisional interaction is strongest. In this region (around $\theta = -13$ in the figure) the $|c|^2$ obtained from eq. 9 becomes complex, clearly indicating the problems in using Shore parameters when PCI is important. However, in the other spectral regions $|c|^2$ approaches the result obtained from eq. 10 and it is our understanding that the quality of the Shore parameter fit is sufficient in these regions. Finally, to study the effect of the experimental resolution on $|c|^2$, we convoluted the theoretical cross section derived from eq. 3 with a Gaussian resolution factor to obtain a more realistic experimental cross section. A typical experimental resolution of 150 meV. was used in the convolution. From the convoluted spectrum, we then used eq. 5 to obtain the Shore parameters and again eq. 9 to find $|c|^2$. As is seen from the figure the c-parameter obtained from the convoluted spectrums does indeed show strong dependence on the electron ejection angle. It is accordingly our understanding that angular dependence of the c-parameter observed by Balashow *et al*, is both an effect of post-collisional interaction, as well as an effect of the experimental resolution.

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[1] V V Balashov, S E Martin and A Crowe, J. Phys B: At. Mol. Opt. (L337-343) 29, 1996
[2] Bruce W. Shore, Reviews of modern physics, 439, 1967
[3] Senashenkov, Sov. Phys. Usp., 1989
[4] M Brauner, J S Bringgs and J T Broad, J. Phys B: At. Mol. Opt. 24)1991) 287-297
[5] M Brauner, J S Bringgs and H Klar, J. Phys. B: At. Mol. Opt. 22 (1989) 2265-2287
[6] U Fano 1961 phys. Rev. 124 1866