E4-2002-140

Yu. V. Popov[1], O. Chuluunbaatar, S. I. Vinitsky,
L. U. Ancarani[2], C. Dal Cappello[2], P. S. Vinitsky[3]

ON THE STUDY OF THE TRANSFER IONIZATION REACTIONS AT SUPER SMALL SCATTERING ANGLES

[1]Nuclear Physics Institute, Moscow State University, Moscow 119992,
 Russia
[2]Institute of Physics, University of Metz, Metz, France
[3]Physics Department, Moscow State University, Moscow 119992,
 Russia

1 Introduction

Recent experiments of Mergel *et al* . [1, 2, 3] have awaken a new wave of interest into the transfer ionization (TI) reactions with fast projectile protons on the helium atom

$$p + He \rightarrow H^0 + He^{2+} + e^-. \qquad (1)$$
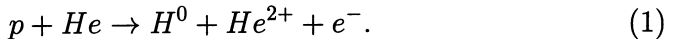
Using the COLTRIMS technique, the momenta of fragments have been measured in coincidence for the first time, and with high resolution, so that the experiment was kinematically complete. The momentum of He^{2+} and the polar and azimuthal scattering angles of the outgoing H atom were measured so that many types of differential cross sections could be obtained.

It is widely believed that a target electron can be captured by a fast-passing proton if their velocities are equal and parallel: one then talks of resonant capture. This conceptual approach led to the so-called Thomas capture mechanisms in which a target electron, after a first collision with the projectile proton, gets the suitable velocity value, and, after a second collision with either the other target electron or with the residual ion, it finally gets the necessary direction to be captured [4]. Such mechanisms correspond to the Thomas peaks in the single differential cross sections which were observed at the predicted scattering angles and projectile energies [1]. However, these well-understood peaks are much smaller in magnitude and situated in a well-defined but different angular domain than the main peak observed by Mergel *et al* . This paper is dedicated to a first step analysis in the interpretation of this new peak.

Since all classical capture mechanisms are not sufficient to describe the cross section observed at small scattering angles [1, 2, 3], we have to turn to pure quantum (off-shell) effects to find an explanation. A quantum approach attributes quantum probabilities to different processes: one can therefore leave aside the strict demand of the parallel motion of fragments with equal velocities and traditional theories for electron capture in high-energy ion-atom collisions can be considered. In this respect it is clear from the early studies [5] that the simple approximations are not able to properly describe the capture

process. For example, the long range character of particles interactions has to be taken into account through distorted waves rather than plane waves. Also, there is the question of when to interrupt the Born series. These and other important issues dealing with the interaction mechanisms are separated from the question of the description of the target ground state which is generally supposed to be of the Hartree-Fock type. However, $(e, 2e)$ and especially $(e, 3e)$ experiments on atoms have demonstrated the essential role played by the electron-electron correlation in the target ground state: simple Hartree-Fock wave functions are not good enough.

In the present paper, we use the Pole Approximation (PA) for proton-atom collision in order to compare the influence of the initial state wave function and we shall consider both uncorrelated and correlated versions. The PA provides us with the most transparent physical picture of the scattering process. The experimental incident proton (projectile) energies are in the range $E_p = 0.15 - 1.4$ MeV [1, 2, 3]. If we prove that the PA is dominant reaction mechanism in this energy domain, we can use this simple model to substantiate TI reaction like the new and effective tool for the angular spectroscopy of electron-electron correlations in the target atom. So, the main aim of this paper is to check up this statement.

Atomic units will be used throughout the paper.

2   Theory

To realize the program formulated above, we write down the exact matrix element of the TI reaction in the *prior* form:

$$\mathcal{T} = <\vec{p}_p \Phi_0 | V_{pHe}[1 + G(E)V_{out}] | \Psi_{out}(\vec{k}, \vec{p}_H, \vec{K}) > . \qquad (2)$$

In (2) $\vec{p}_p$ is the proton momentum, $\vec{k}$ the momentum of the escaped electron, $\vec{p}_H$ the hydrogen momentum, $\vec{K}$ the ion momentum, $V_{pHe} = V_{pe_1} + V_{pe_2} + V_{Np}$ and $G(E) = (E - \mathcal{H} + i\varepsilon)^{-1}$ is the total Green function. The final state wave function $|\Psi_{out}>$ satisfies the equation

$$(E - \mathcal{H} + V_{out})|\Psi_{out}> = 0 \qquad (3)$$

2

with V_{out} being the potential in the final state. The choice of this potential is rather arbitrary and a matter of physical model. We choose it like $V_{out} = V_{ee} + V_{Np}$ to keep in a simple way all necessary symmetries. In this particular case $|\Psi_{out}>$ presents the wave function of two non-interacting electrons in the field of two moving charged centers [6]. This function is quite complex, therefore we consider only its symmetrized asymptotic form

$$< \vec{r}_p, \vec{r}_1, \vec{r}_2, \vec{r}_N |\Psi_{out}(\vec{k}, \vec{p}_H, \vec{K}) >\approx$$

$$N[e^{-i\vec{p}_H \vec{R}_{p1}}\varphi_H(\vec{\rho}_{p1})e^{-i(\vec{K}+\vec{k})\vec{R}_{N2}}\varphi_{He^{++}}^{-*}(\vec{\rho}_{N2}, \frac{\vec{K} - M\vec{k}}{M+1}) + (1 \leftrightarrow 2)] \quad (4)$$

with

$$\vec{R}_{pi} = \frac{m\vec{r}_p + \vec{r}_i}{m+1}; \quad \vec{\rho}_{pi} = \vec{r}_p - \vec{r}_i; \quad m = 1836.15 \text{ is proton mass,}$$

and, consequently,

$$\vec{R}_{Ni} = \frac{M\vec{r}_N + \vec{r}_i}{M+1}; \quad \vec{\rho}_{Ni} = \vec{r}_N - \vec{r}_i; \quad M \approx 4m \ .$$

Also it is possible to show that at rather large proton velocity v_p, $N \approx 1/\sqrt{2}$.

All terms which really can present more or less direct information on a target atom wave function [7] are contained in the first Born term (FBA) of (2). Any additional rescattering in the second or higher Born terms disperses the valuable information on the target wave function because of an integration over its coordinates. The FBA with the function (4) takes the form

$$\mathcal{T}_{FBA} = -4\pi\sqrt{2} \int \frac{d\vec{x}}{(2\pi)^3} \frac{\tilde{\varphi}_H(\vec{x})}{|\vec{v}_p - \vec{q} - \vec{x}|^2}[F(\vec{q}; 0; \vec{k}) + F(\vec{v}_p - \vec{x}; -\vec{v}_p + \vec{q} + \vec{x}; \vec{k})$$

$$-2F(\vec{v}_p - \vec{x}; 0; \vec{k})], \quad (5)$$

where

$$F(\vec{y}; \vec{\eta}; \vec{k}) = \int e^{-i\vec{y}\vec{r}_1 - i\vec{\eta}\vec{r}_2}\varphi^{-*}(\vec{k}, \vec{r}_2)\Phi_0(\vec{r}_1, \vec{r}_2)d\vec{r}_1 d\vec{r}_2$$

3

$$= \int \frac{d\vec{\xi}}{(2\pi)^3} \tilde{\varphi}^{-*}(\vec{k}, \vec{\xi}) \widetilde{\Phi}_0(\vec{y}, \vec{\eta} + \vec{\xi}). \tag{6}$$

In (5) $\vec{q} = \vec{p}_H - \vec{p}_p$ is the transferred momentum, and tilde means the momentum representation. The hydrogen wave function satisfies the Schrödinger equation

$$(E_0{}^H - \frac{x^2}{2})\tilde{\varphi}_H(\vec{x}) = \int \frac{d\vec{x}'}{(2\pi)^3} \frac{-4\pi}{|\vec{x} - \vec{x}'|^2}\tilde{\varphi}_H(\vec{x}') \tag{7}$$

whose normalized solution is well known:

$$\tilde{\varphi}_H(\vec{x}) = \frac{8\sqrt{\pi}}{(1 + x^2)^2}. \tag{8}$$

From (5) and (8) we obtain

$$\mathcal{T}_{PA} = -\frac{4\sqrt{2\pi}}{1 + |\vec{v}_p - \vec{q}|^2} F(\vec{q}; 0; \vec{k}). \tag{9}$$

It is the first term in the sum (5) which presents the PA. This term can be displayed in a diagram form:
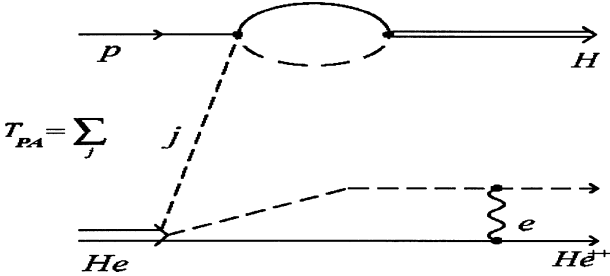

Figure 1: The diagram image of the Pole Approximation

What is the transferred momentum vector $\vec{q}$? According to the momentum and energy conservation we have the following equations in the laboratory coordinate system:

$$\vec{K} + \vec{k} + \vec{q} = 0, \tag{10}$$

4

$$E = \frac{p_p^2}{2m} + E_0^{He} = \frac{p_H^2}{2(m+1)} + \frac{k^2}{2} + \frac{K^2}{2M} + E_0^H. \qquad (11)$$

In (10) and (11) $E_0^{He} = -2.903$ and $E_0^H = -0.5$. For conveniency we put $Q = E_0^{He} - E_0^H = -2.403$.

In the experiment $E_p = 0.15 \div 1.4$ MeV, i.e. $v_p = 2.45 \div 7.49$. At the same time the measured transferred and ion momenta are of the order of a few atomic units at super small angles $\theta_p = 0.1 \div 0.5$ mrad, which allows one to neglect $K^2/2M$ and $q^2/2m$ in (11), because of very large masses m and M. We have to emphasize that one can do it only at very small scattering angles θ_p when the interaction between the proton and the ion takes place practically due to a transferred electron. As a result of these approximations we have

$$\vec{v}_p \vec{q} = \frac{1}{2} v_p^2 - \frac{1}{2} k^2 + Q. \qquad (12)$$

If we choose the z axis along the vector $\vec{v}_p$, then $\vec{q} = (\vec{q}_\perp, q_z)$ with

$$q_z = \frac{v_p}{2} - \frac{k^2 - 2Q}{2v_p} \qquad (13)$$

and $q_\perp \approx m v_p \theta_p$. So, the momentum of the transferred (captured) electron is

$$\vec{k}_1 \equiv \vec{q} = (m v_p \theta_p, 0, q_z). \qquad (14)$$

3 Results and Discussion

We used the correct eq. (9) for calculations of the singly differential cross section

$$\frac{d\sigma}{d\theta_p} = \frac{m^2 \theta_p}{(2\pi)^4} \int |\mathcal{T}_{PA}|^2 d\vec{k} \qquad (15)$$

which was measured by the HSB experimental team [1]. Three different helium wave functions were taken for calculations:
- the simplest Hylleraas function [8]

$$\Phi_0(\vec{r}_1, \vec{r}_2) = \frac{Z^3}{\pi} e^{-Z(r_1 + r_2)}, Z = 27/16$$

(we refer to it as Hy);
- the best function of Bonham and Kohl [9] (number 17, referred to as BK);
- non-coupled twelve-component correlated variational function [10] (referred to as CPV) generated specially for this paper.

We remind that to get the non-coupled correlated variational function the set of helium coordinates

$$s = r_1 + r_2, \quad v = r_{12}/(r_1 + r_2), \quad w = (r_1 - r_2)/r_{12}$$

is used instead of the well-known Hylleraas set

$$s = r_1 + r_2, \quad t = r_1 - r_2, \quad u = r_{12} = |\vec{r_1} - \vec{r_2}|.$$

The helium wave function takes the form

$$\Phi_0(s, v, w) = \sum_{i,j,k=0} C_{i,j,2k} U_i(s) V_j(v) W_{2k}(w) \tag{16}$$

with

$$U_i(s) = N_i e^{-\alpha_i s} L_i^5(2\alpha_i s), \quad V_j(v) = \overline{N}_j P_j^{(0,2)}(2v - 1),$$
$$W_{2k}(w) = \hat{N}_{2k} P_{2k}^{(1,1)}(w). \tag{17}$$

In (17)

$$N_i = \sqrt{\frac{i!(2\alpha_i)^6}{(i+5)!}}, \quad \overline{N}_j = \sqrt{2j+3}, \quad \hat{N}_{2k} = \sqrt{\frac{(k+1)(4k+3)}{2(2k+1)}} \tag{18}$$

are the normalization constants, L_i^5 are the generalized Laguerre polynomials, $P_j^{(q,t)}$ are the Jacobi polynomials and α_i are the variational parameters. With only a single parameter α the basis functions are orthonormal:

$$\int_0^\infty s^5 U_n(s) U_m(s) ds = \delta_{n,m}, \quad \int_0^1 v^2 V_n(v) V_m(v) dv = \delta_{n,m},$$

$$\int_0^1 (1 - w^2) W_{2n}(w) W_{2m}(w) dw = \delta_{n,m}.$$

In the CPV function the only parameter $\alpha = 1.7 \approx \sqrt{-E_0^{He}}$ is used which determines amount 12 of terms in (16).
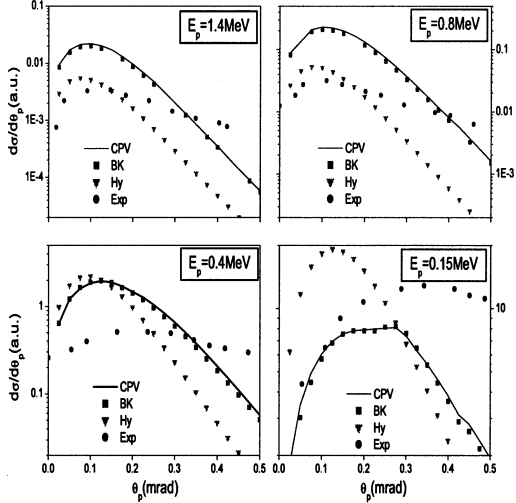
6

Figure 2: Singly differential cross section $d\sigma/d\theta_p$ for the reaction $p + He \rightarrow H + e + He^{++}$ at four different proton energies. The experimental points are taken from [1]

We would like to focus our attention on a few features of the considered reaction. Firstly, the value $v_p \sim 7$ on the upper limit of proton energies allows one to consider the velocity v_p as a large parameter. But even the proton energy $E_p = 1.4$ MeV is not large enough to consider it as asymptotically large. Secondly, one can easily show that for the simplest Hy function the value $F(\vec{q}; 0; \vec{k}) \sim v_p^{-4}$. More correlated wave functions give the same order of magnitude. However, if we estimate another FBA, or SBA terms in (2), or calculate more carefully the two-center function $|\Psi_{out}>$ in (4), then we can see that these additional terms are of the same order as $\mathcal{T}_{PA}$. This means that even for asymptotically large v_p the term $\mathcal{T}_{PA}$ does not approximate the experiment.

The manifestation of these features we just observe on Fig.2. It is evident that: 1) absolute peak values even at $E_p = 1.4$ MeV are approximately 6 times higher than the experiment; 2) the peaks of

calculated curves are noticably shifted to the side of smaller angles θ_p; 3) experimental points after peak fall down much slower than calculations.

Of course, the results of calculations differ for correlated and non-correlated helium wave functions, but for both cases the coincidence to the experiment is very poor. This means that to describe the experiment we have to factor out and sum up all terms of the order v_p^{-4} and, perhaps, v_p^{-5}. But in this case the reaction $p + A \rightarrow H + e + A^{++}$ is no longer useful for the purposes of angular spectroscopy of the electron-electron correlations in target atom.

References

[1] V. Mergel, Ph.D. thesis, Univ. Frankfurt/Main, Shaker Verlag, 1996.

[2] V. Mergel *et al.*, Phys. Rev. Lett. **79**, 387 (1997).

[3] V. Mergel *et al.*, Phys. Rev. Lett. **86**, 2257 (2001).

[4] L.H. Thomas, Proc. R. Soc. London Ser. B **114**, 561 (1927).

[5] Dz. Belkić, R. Gayet and A. Salin, Phys. Rep. **56**, 279 (1979).

[6] E.A. Solov'ev and S.I. Vinitsky, J.Phys. B **18**, L567 (1985).

[7] V.G. Neudatchin, Yu.V. Popov and Yu.F. Smirnov, Physics Uspekhi **42**, 1017 (1999); Yu.V. Popov, C. Dal Cappello and K. Kouzakov, J. Phys. B **29**, 5901 (1996).

[8] H.A. Bethe, E.E. Salpeter, "Quantum mechanics of one and two electron atoms", Springer-Verlag, Berlin, 1957.

[9] R.A. Bonham and D.A. Kohl, J. Chem. Phys. **45**, 2471 (1966).

[10] O. Chuluunbaatar et al. J. Phys. B **34**, L425 (2001).

Попов Ю. В. и др.   Е4-2002-140
Исследование реакций захвата с ионизацией
при сверхмалых углах рассеяния

Рассмотрена гипотеза о том, что реакцию $p + \text{He} \rightarrow \text{H} + \text{He}^{++} + e$ при сверхмалых углах рассеяния водорода можно использовать для целей угловой спектроскопии электронных корреляций в мишени. Показана несостоятельность этой гипотезы.

Работа выполнена в Лаборатории информационных технологий ОИЯИ.

Popov Yu. V. et al.   Е4-2002-140
On the Study of the Transfer Ionization Reactions
at Super Small Scattering Angles

The hypothesis that the reaction $p + \text{He} \rightarrow \text{H} + \text{He}^{++} + e$ at super small scattering angles of hydrogen can be used for purposes of the angular spectroscopy of electron-electron correlations in the target is considered. It is shown that this hypothesis is insolvent.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

Редактор *Е. И. Кравченко*
Макет *Е. В. Сабаевой*