

ATOMS, SPECTRA,
 RADIATION

**Theoretical Investigation of the $p + \text{He} \rightarrow \text{H} + \text{He}^+$
 and $p + \text{He} \rightarrow \text{H} + \text{He}^{++} + e$ Reactions
 at Very Small Scattering Angles of Hydrogen**

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Abstract—A hypothesis is considered that the reactions $p + \text{He} \rightarrow \text{H} + \text{He}^+$ and $p + \text{He} \rightarrow \text{H} + \text{He}^{++} + e$ at very small scattering angles of hydrogen can be used for the angular spectroscopy of electron correlations in a target. It is shown that this hypothesis is inconsistent. © 2002 MAIK “Nauka/Interperiodica”.

1. INTRODUCTION

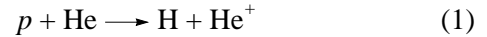
A number of sufficiently fine experiments have been carried out over the last several years on the capture of an electron by a fast proton from a helium target, including those with a simultaneous transfer ionization process. With the use of a unique cold target recoil ion momentum spectroscopy (COLTRIMS), all independent kinematic characteristics of the final products of reactions were measured: the polar and azimuthal angles of hydrogen, as well as the momentum and energy of a He^{++} ion [1–3]. The azimuthal scattering angle θ_p of hydrogen was as small as 0.1–0.5 mrad, which is about 100 times less than that obtained in earlier experiments of this type. The proton energy E_p ranged from 0.15 to 1.4 MeV.

The singly differential cross section $d\sigma/d\theta_p$ of these reactions in the range of θ_p from 10 to 1000 mrad represents a sufficiently smoothly and rapidly decreasing function, which is satisfactorily described within the continuum distorted wave formalism [4, 5]. At angles of $\theta_p = 0.1$ –0.3 mrad, this curve attains its principal maximum (not counting relatively small Thomas peaks at appropriate scattering angles [6, 7] greater than 0.5 mrad).

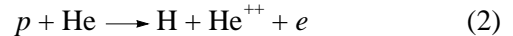
The authors of the experimental works [1–3] suggested that the reaction $p + \text{He} \rightarrow \text{H} + \text{He}^{++} + e$ in this range of extremely small scattering angles θ_p can be used for obtaining new and extraordinary information on the structure of the wave function of the target in the momentum representation. The present paper is devoted to the theoretical analysis of this concept. Throughout this paper, we use atomic units.

2. THEORY

For brevity, we will call the reaction



a simple capture (SC) reaction and



a transfer ionization (TI) reaction. We will also use the following notation: $\mathbf{v}_p(\mathbf{p}_p)$ is the proton velocity (momentum), $\mathbf{v}_H(\mathbf{p}_H)$ is the hydrogen velocity (momentum), \mathbf{k} is the momentum of the escaped electron, \mathbf{K} is the momentum of the residual ion, and E is the total energy of the system. In atomic units, the proton mass is $m = 1836.15$ and the ion mass is $M \approx 4m$. In addition, we introduce the transferred momentum

$$\mathbf{q} = \mathbf{p}_H - \mathbf{p}_p = (m + 1)\mathbf{v}_H - m\mathbf{v}_p.$$

First, consider the TI reaction. In the notation introduced, the energy and momentum conservation laws in the laboratory system of coordinates are expressed as

$$\mathbf{K} + \mathbf{k} + \mathbf{q} = 0 \quad (3)$$

and

$$E = \frac{p_p^2}{2m} + E_0^{\text{He}} = \frac{p_H^2}{2(m+1)} + \frac{k^2}{2} + \frac{K^2}{2M} + E_0^{\text{H}}, \quad (4)$$

respectively. Here, $E_0^{\text{He}} = -2.903$ and $E_0^{\text{H}} = -0.5$. For convenience, we introduce the quantity $Q = E_0^{\text{He}} - E_0^{\text{H}} = -2.403$.

The proton energy E_p ranges from 0.15 to 1.4 MeV, which corresponds to $v_p = 2.45$ –7.49. At the same time,

it follows from the experiments that the measured values of the ion momentum and the transferred momentum at very small angles θ_p only amount to a few atomic units; this fact allows one to neglect the energies $K^2/2M$ and $q^2/2m$ as compared with other terms in Eq. (4). We stress that this can only be done at very small angles $\theta_p = 0.1\text{--}0.5$ mrad, when the helium ion remains at rest. At larger scattering angles, the proton–nucleon (pN) Coulomb interaction begins to play an increasing role, which significantly increases the transferred momentum and the momentum of the residual ion, which starts to move. Under the approximations made, it follows from (4) that

$$\mathbf{v}_p \mathbf{q} = \frac{1}{2} v_p^2 - \frac{1}{2} k^2 + Q. \quad (5)$$

If we choose the proton velocity vector as the z axis, we have $\mathbf{q} = (\mathbf{q}_\perp, q_z)$, where

$$q_z = \frac{v_p}{2} - \frac{k^2 - 2Q}{2v_p} \quad (6)$$

and $q_\perp = m v_p \sin \theta_p \approx m v_p \theta_p$. Note in passing that Eqs. (3)–(5) allow one to determine the total momentum of the electron provided that the momentum of the ion has been measured, to obtain appropriate constraints, etc.

For the SC reaction, Eqs. (3) and (4) are rewritten as

$$\mathbf{K} + \mathbf{q} = 0 \quad (7)$$

and

$$\frac{p_p^2}{2m} + E_0^{\text{He}} = \frac{p_H^2}{2(m+1)} + \frac{K^2}{2(M+1)} + E_0^{\text{H}} + E_0^{\text{He}^+}, \quad (8)$$

where $E_0^{\text{He}^+} = -2$. Here, it is convenient to introduce a quantity $Q' = E_0^{\text{He}} - E_0^{\text{H}} - E_0^{\text{He}^+} = -0.403$. Equation (6) is modified as follows:

$$q_z = \frac{v_p}{2} + \frac{Q'}{v_p}. \quad (9)$$

Now, we pass on to the dynamics of the processes. Let us write the Hamiltonian of the system $p + \text{He}$ as

$$\mathcal{H} = \mathcal{H}_p + \mathcal{H}_{\text{He}} + V_{p\text{He}}, \quad (10)$$

where

$$\begin{aligned} \mathcal{H}_p &= p_p^2/2m, \\ \mathcal{H}_{\text{He}} &= k_1^2/2 + k_2^2/2 + V_{Ne_1} + V_{Ne_2} + V_{ee}, \\ V_{p\text{He}} &= V_{pe_1} + V_{pe_2} + V_{Np}, \\ V &= V_{p\text{He}} + V_{Ne_1} + V_{Ne_2} + V_{ee}. \end{aligned} \quad (11)$$

Next, we use the following notation: $|\Phi_0\rangle$ is the wave function of the helium atom at rest in the ground state;

$|\mathbf{p}_H, \Phi_H\rangle$ is the wave function of the hydrogen atom in the ground state that moves at velocity \mathbf{v}_N ; and $|\mathbf{K}, \varphi(\mathbf{k})\rangle$ is the wave function of the electron in the field of the ion He^{++} with momentum \mathbf{K} (in the case of the SC reaction, one should take the function $|\varphi_0\rangle$ of the bound electron instead of $|\varphi(\mathbf{k})\rangle$).

We consider a helium atom in a singlet state; therefore, it is convenient to represent the amplitude of the TI reaction with regard to all the necessary symmetries as follows:

$$\mathcal{T} = \langle \mathbf{p}_p \Phi_0 | V_{p\text{He}} [1 + G(E) V_{\text{out}}] | \Psi_{\text{out}} \rangle, \quad (12)$$

where

$$G(E) = (E - \mathcal{H}_p - \mathcal{H}_{\text{He}} - V + i\varepsilon)^{-1}$$

is the full Green's function of the problem and $|\Psi_{\text{out}}\rangle$ is determined from the equation

$$[E - H_0 - (V - V_{\text{out}})] |\Psi_{\text{out}}\rangle = 0,$$

where $V_{\text{out}} = V_{ee} + V_{pN}$.

The amplitude (12) is exact, and the final state represents the wave function of two noninteracting electrons in the field of two centers that move relative to each other. Here, we consider the approximation of this complicated function by its asymptotic value, i.e., by the normalized combination of functions

$$\langle \mathbf{r}_p, \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_N | \mathbf{p}_H, \Phi_H; \mathbf{K}, \varphi^-(\mathbf{k}) \rangle,$$

which is symmetric with respect to the electron coordinates. Even this simplification leaves open the problem of correct normalization, which requires the orthogonalization of all components. However, considering the velocity v_p as a large parameter in the problem, one can neglect the cross-terms in the normalization integral and obtain an approximate normalization factor of $N = 1/\sqrt{2}$.

Formula (12) clearly shows that the term in the first Born approximation in $V_{p\text{He}}$ in problems with rearrangement is largely determined by the choice of the output potential V_{out} , i.e., by the interaction in the final state; therefore, this term does not provide a suitable approximation for the amplitude \mathcal{T} even for a large energy E . However, we will consider this term because it is this term that includes the simplest mechanism when one electron is captured immediately by a proton from an atom, while the other is emitted by the He^+ ion due to the shake-off process of the internal electric field in the atom. Indeed, leaving only $V_{p\text{He}}$ in (12) and calculating the matrix element, we obtain

$$\begin{aligned} \mathcal{T}_0 &= -4\pi\sqrt{2} \int \frac{d\mathbf{x}}{(2\pi)^2} \frac{\tilde{\Phi}_H(\mathbf{x})}{|\mathbf{v}_p - \mathbf{q} - \mathbf{x}|^2} [F(\mathbf{q}; 0; \mathbf{k}) \\ &+ F(\mathbf{v}_p - \mathbf{x}; -\mathbf{v}_p + \mathbf{q} + \mathbf{x}; \mathbf{k}) - 2F(\mathbf{v}_p - \mathbf{x}; 0; \mathbf{k})], \end{aligned} \quad (13)$$

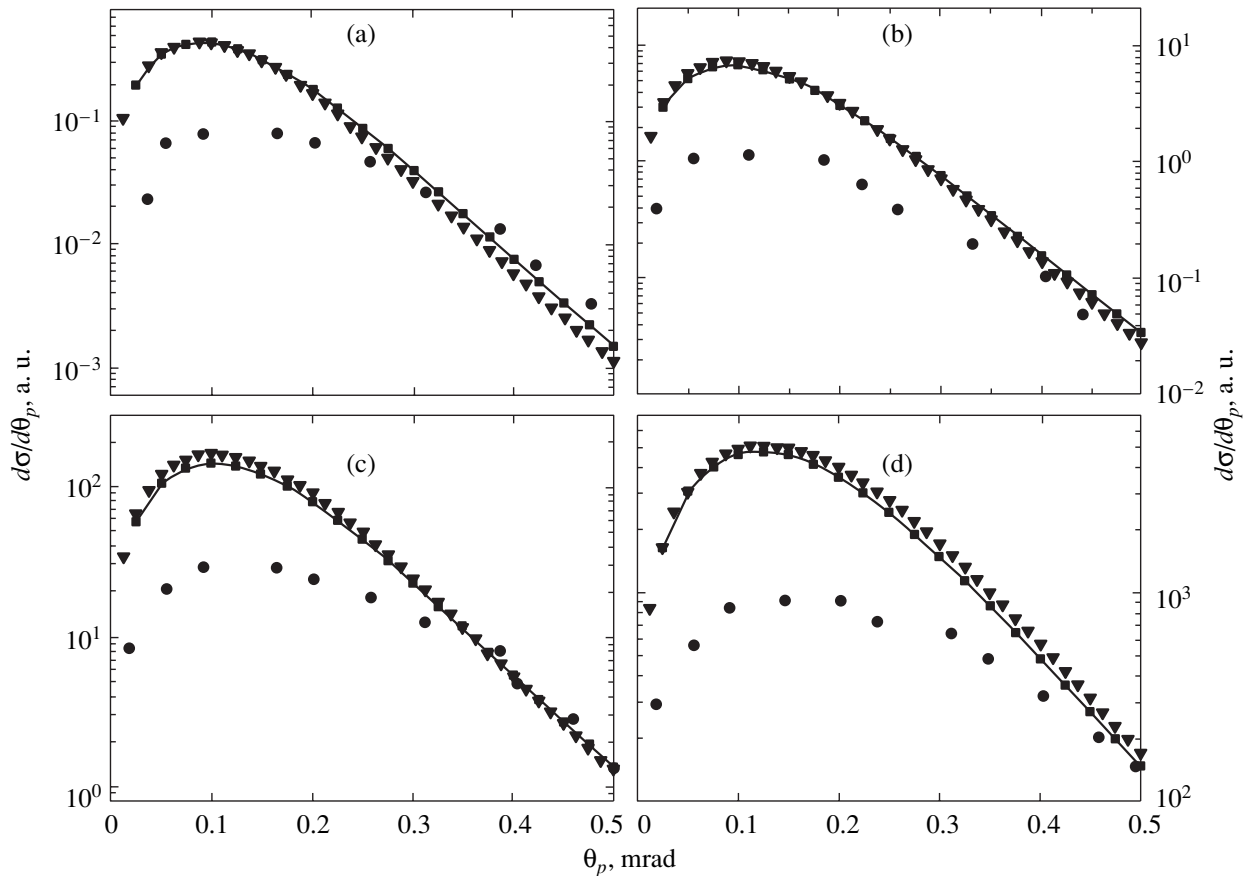


Fig. 1. Singly differential cross section $d\sigma/d\theta_p$ for the reaction $p + \text{He} \rightarrow \text{H} + \text{He}^+$ calculated with the use of the following functions: (solid curve) CVP, (squares) BK, and (triangles) Hy for four different values of the collision energy E_p : (a) 1.4, (b) 0.8, (c) 0.4, and (d) 0.15 MeV. Relative error of the experiment (circles) in case (a) is no greater than 10% in the range of angles considered.

where

$$\begin{aligned}
 F(\mathbf{y}; \boldsymbol{\eta}; \mathbf{k}) &= \int \exp(-i\mathbf{y} \cdot \mathbf{r}_1 - i\boldsymbol{\eta} \cdot \mathbf{r}_2) \\
 &\times \varphi^{-*}(\mathbf{k}, \mathbf{r}_2)\Phi_0(\mathbf{r}_1, \mathbf{r}_2)d\mathbf{r}_1d\mathbf{r}_2 \\
 &= \int \frac{d\xi}{(2\pi)^3} \tilde{\varphi}^{-*}(\mathbf{k}, \xi)\tilde{\Phi}_0(\mathbf{y}, \boldsymbol{\eta} + \xi)
 \end{aligned}
 \tag{14}$$

(the tilde over the functions denotes the momentum representation of these functions). Invoking the equation for the hydrogen wave function in the momentum representation,

$$\left(E_0^{\text{H}} - \frac{x^2}{2}\right)\tilde{\varphi}_{\text{H}}(\mathbf{x}) = \int \frac{d\mathbf{x}'}{(2\pi)^3} \frac{-4\pi}{|\mathbf{x} - \mathbf{x}'|^2} \tilde{\varphi}_{\text{H}}(\mathbf{x}'), \tag{15}$$

whose normalized solution

$$\tilde{\varphi}_{\text{H}}(\mathbf{x}) = \frac{8\sqrt{\pi}}{(1 + x^2)^2} \tag{16}$$

is well known, we obtain

$$\mathcal{T}_0^{(1)} = -\frac{4\sqrt{2\pi}}{1 + |\mathbf{v}_p - \mathbf{q}|^2} F(\mathbf{q}; 0; \mathbf{k}). \tag{17}$$

This is nothing but the first term in the sum (13), which corresponds to the shake-off process described above. Note that the electron captured by a proton has momentum \mathbf{q} , and the process described by formula (17) is a purely quantum one, which has nothing to do with the classical resonant capture. The second term in (13) represents the exchange term, and the third term corresponds to the Coulomb interaction of a proton with the nucleus in the first Born approximation.

Here, we restrict our attention to the amplitude (17) since the quantity

$$\begin{aligned}
 F(\mathbf{q}; 0; \mathbf{k}) &= \int \exp(-i\mathbf{q} \cdot \mathbf{r}_1) \\
 &\times \varphi^{-*}(\mathbf{k}, \mathbf{r}_2)\Phi_0(\mathbf{r}_1, \mathbf{r}_2)d\mathbf{r}_1d\mathbf{r}_2
 \end{aligned}
 \tag{18}$$

represents the Fourier transform of the coordinate wave function of the helium atom; according to the hypothesis of the authors of the experiments, it is this term that should dominate in the general amplitude (12) and pro-

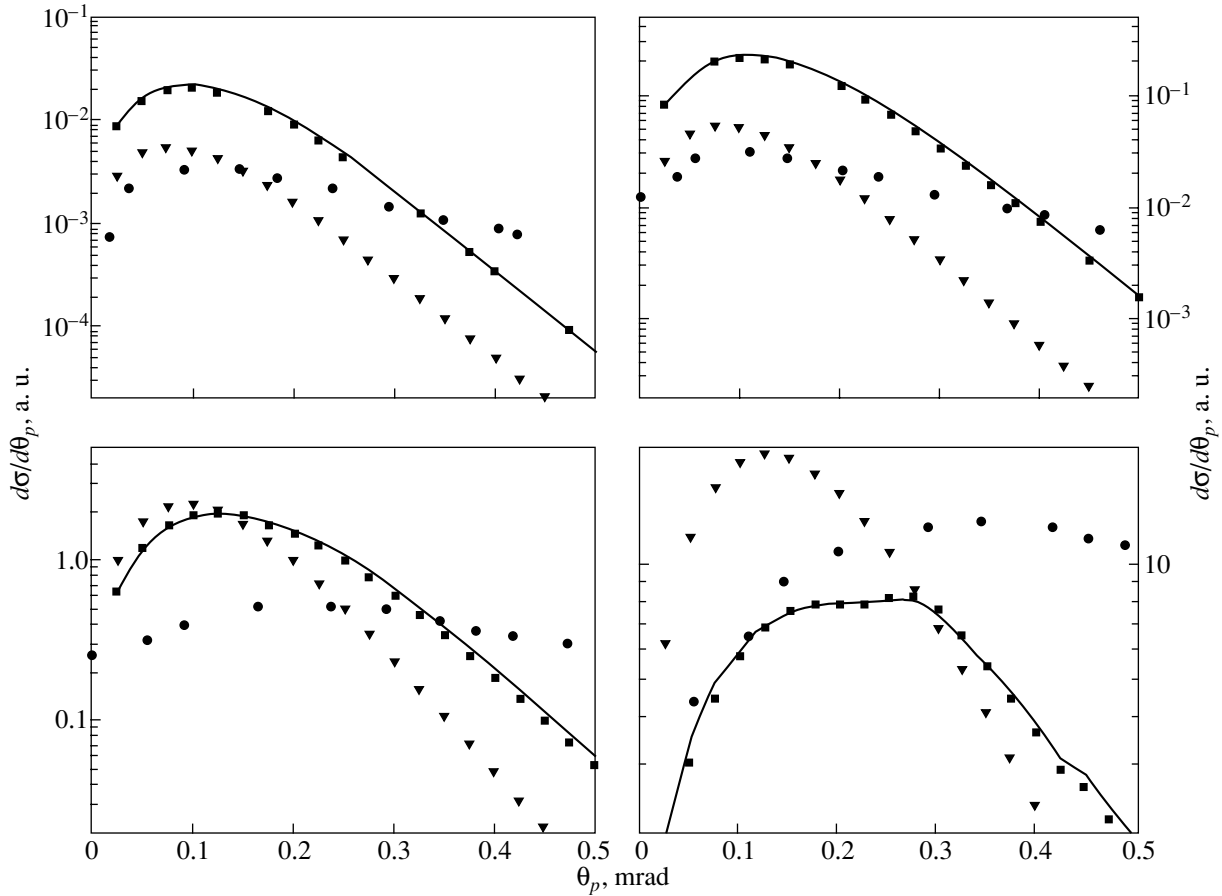


Fig. 2. Same as in Fig. 1 for the reaction $p + \text{He} \rightarrow \text{H} + e + \text{He}^{++}$. Relative error of the experiment (circles) in case (a) is no greater than 20% in the range of angles considered.

vide information on the correlation structure of the wave function $\Phi_0(\mathbf{r}_1, \mathbf{r}_2)$ in the range of very small angles θ_p . Note that a function of type (18) appears in the amplitude of the process ($e, 3e$) [8, 9]; it was demonstrated that this process provides a powerful tool for the angular spectroscopy of $e-e$ correlations in the target under investigation.

In the case of the SC reaction, the amplitude is given by (17); however, one should replace the amplitude $\varphi^{-*}(\mathbf{k}, \mathbf{r})$ in integral (18) by $\varphi_0(r) = \sqrt{(8/\pi)} \exp(-2r)$.

The differential cross section of the TI process is represented as

$$d^5\sigma = \frac{|\mathcal{T}|^2}{v_p^2} \frac{d\mathbf{q}_\perp}{(2\pi)^2} \frac{d\mathbf{k}}{(2\pi)^3} = \frac{m^2}{(2\pi)^5} |\mathcal{T}|^2 d\Omega_H d\mathbf{k}. \quad (19)$$

The singly differential cross section, which we calculated, follows from (19):

$$\frac{d\sigma}{d\theta_p} = \frac{m^2 \theta_p}{(2\pi)^4} \int |\mathcal{T}|^2 d\mathbf{k}. \quad (20)$$

For the SC reaction, formula (20) reduces to

$$\frac{d\sigma}{d\theta_p} = \frac{m^2 \theta_p}{2\pi} |\mathcal{T}|^2. \quad (21)$$

3. RESULTS OF CALCULATIONS AND DISCUSSION

Figures 1 and 2 represent the calculated cross sections (20) and (21) with the amplitude $\mathcal{T}_0^{(1)}$. In these calculations, we used the following three functions $\Phi_0(\mathbf{r}_1, \mathbf{r}_2)$:

- (1) the simplest of the Hylleraas functions [10]

$$\Phi_0(\mathbf{r}_1, \mathbf{r}_2) = \frac{Z^3}{\pi} \exp[-Z(r_1 + r_2)], \quad Z = \frac{27}{16}$$

(indicated by the symbol Hy);

- (2) one of the best functions of Bonham and Kohl [11] (number 17, denoted by BK);

(3) the factorized 12-component correlated variational function [12], denoted by CVP, which was designed by the authors specially for the present study. The experimental results are borrowed from [1].

We should immediately point out several features of the processes considered. First, the value $v_p \approx 7$ in the upper limit of the range of proton energies allows us to treat the proton velocity as a large parameter in the problem. The transferred momentum $q \geq v_p/2$ also is a large parameter; this fact distinguishes the capture reaction from the reactions ($e, 2e$) and ($e, 3e$), where this parameter is small ($q \sim 0-2$). On the other hand, if, by analogy with the processes ($e, 2e$) and ($e, 3e$), we calculate the velocity v_p for the energy of the initial electron, then this energy will correspond to 700 eV in the upper limit, which is obviously insufficient for the impulse approximation.

Second, one can easily show that $\mathcal{T}_0^{(1)} \propto v_p^{-6}$ in the case of a simple separable function Hy. Other, more correlated, functions also have the same order of smallness. However, if we analyze (at least qualitatively) the second Born approximation [13], or more accurately calculate the two-center function Ψ_{out} in (12), then we can see more terms of the same order. Thus, one should not expect that $\mathcal{T}_0^{(1)}$ is a suitable approximation even for asymptotically large v_p .

These features are manifested in the figures. In the case of the SC reactions, all the calculated results virtually coincide but appreciably differ from the experimental results: (1) the absolute values in the maximum for $E_p = 1.4$ MeV differ approximately by a factor of six; (2) the maximum itself is shifted toward smaller scattering angles; and (3) the shapes of the curves do not coincide (the experimental curve decays much more slowly after the maximum).

The same applies to the TI reactions, although the results of calculations for correlated and uncorrelated functions are different, as was to be expected.

The comparison of the theoretical and experimental results shows that, even for very small angles when the amplitude $\mathcal{T}_0^{(1)}$ seems to dominate and carry certain exclusive information on electron–electron correlations in the target, corrections due to other mechanisms in the first and second Born approximations are sufficiently large so that the reaction $p + A \rightarrow H + e + A^{++}$ cannot be considered useful for the method of angular spectroscopy of correlations.

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