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FOUR-BODY ONE-CHANNEL DISTORTED-WAVE THEORIES FOR SINGLE ELECTRON TRANSFER

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Abstract. *The two versions of the Born distorted wave (BDW) models are formulated within the framework of the four-body scattering theory. As an illustration the BDW approximation is applied to compute the differential cross sections for a single charge exchange in p + H e collision at 500 keV. The present calculated results are found to be in good agreement with experimental data.*

1. INTRODUCTION

The dynamics of the entangled many-body atomic systems is still one of the most fundamental challenges in physics. Since the helium atom is the simplest many-electron system, the investigation of the four-particle $p + He$ collision process has attracted particular interest from both the experimental and the theoretical sides. The experimental data for the differential cross sections (DCS) in $p + He$ collisions have been measured by Martin *et al* [1] for incident proton energies of 25, 30, 50 and 100 keV and by Bratton *et al* [2] for the energy 293 keV. Horsdal-Pedersen *et al* [3] have been reported experimental DCS for electron capture by proton of 2.82, 5.42 and 7.40 MeV from He. These authors reported experimental detection of a peak in the angular distribution for high-velocity. This peak occurs near 0.47 $mrad$ and has been interpreted as the first experimental detection of the Thomas peak in electron capture. Electron capture at high velocity has been understood as a two-step process where the electron makes the transition from its initial to final state by passing through an intermediate state. This picture originated with Thomas [4] who proposed a classical model where capture occurs in two steps.

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In a recent work Mergel *et al* [5] using the Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS) technique have measured the DCS for the four-body process of the proton-helium electron capture at ten impact energies between 150 and 1400 keV. The electron capture can proceed via various reaction channels: (i) electron-electron Thomas, (ii) nucleus-electron Thomas, and (iii) kinematical capture.

Thus far, the DCS for $p + He$ collisions have been theoretically evaluated by means of different methods. For example, the three-body continuum distorted wave (CDW-3B) model was applied by Belkić and Salin [6] in $p+He$ collisions at 293 keV. They clearly showed the discrepancy between DCS obtained with and without the Coulomb internuclear repulsion. The same method was used by Rivarola *et al* [7,8] for calculating the DCS at higher impact energies (2.82, 5.42 and 7.40 MeV). The second Born approximation employing a free-particle Green function has been used in refs. [9,10]. At high energies the DCS for capture in $p + He$ collisions have also been calculated by means of a second-order Faddeev scattering formalism [11], as well as by the strong potential Born method [12]. The calculations of the DCS at intermediate energies by means of the close-coupling method have been carried out by Slim *et al* [13] and Martin *et al* [1]. All of the above quoted theoretical approaches are within the framework of the independent-electron model (IEM), where a given 'active' electron is assumed to evolve independently of the other in the Coulomb field of colliding heavy nuclei screened by a static potential of the other 'passive' electron. The main limitation of IEM lies in the inclusion of electron-electron interaction, and so the model is expected to provide a good description of the collision process where the correlated motion of the electrons are negligible in the collision. At the same time as it is well known that it is very difficult to treat the many-electron problem when all interactions are included in the calculation. Such treatment allows one to study in detail the effect of the electron-electron correlation, and, therefore, to test the approximations introduced in the independent electron model. Among the very few studies along this directions more recently the Born Distorted Wave (BDW) model has been devised to include all interactions in the four-body treatment [14,15].

The BDW approach is a one-channel distorted wave model which exactly coincides with four body Continuum Distorted Wave (CDW-4B) theory [16-18] in the entrance channel and with the four-body corrected first Born (CB1-4B) approximation [19,20] in the exit channel. The associated perturbation potential in the prior transition amplitude coincides with corresponding quantity of the CDW-4B model. Hence, the captured electron is treated in an asymmetrical manner in the entrance and exit channels. The BDW method takes account of the Coulomb continuum

intermediate state of the captured electron only in the entrance channel, since according to the CB1-4B model, captured electron is free in the intermediate stage of collision. The BDW model preserves the four-body nature of the problem and satisfies the correct boundary conditions in the entrance and exit channels.

In the present work the numerical computations of the differential cross sections for single electron capture in $p + He$ collisions are performed at $500\,keV$ by means of BDW theory. The validity of the proposed theoretical results is assessed in comparison with the available experimental data.

Atomic units will be used throughout, expect where otherwise stated.

2. Theory

The single charge exchange from a two-electron atom or ion by a bare projectile may be written as:

$$Z_P + (Z_T; e_1, e_2)_i \longrightarrow (Z_P; e_1)_{f_1} + (Z_T; e_2)_{f_2}, \tag{2.1}$$

where Z_P and Z_T are respectively the charges of the projectile and the target. The indices i and f_1, f_2 label the initial and final bound states respectively. Let $\vec{x}_j$ ($\vec{s}_j$) be the relative vector of the jth electron with respect to the nucleus of the target (projectile) ($j = 1, 2$). The internuclear vector directed from the target nucleus to the projectile nucleus will be denoted by $\vec{R}$, whereas the distance between the electrons is given by r_{12}.

In the entrance channel, it is convenient to introduce $\vec{r}_i$ as a relative vector of Z_P with respect to the center of mass of $(Z_T; e_1, e_2)$. Symmetrically, $\vec{r}_f$ will denote the relative vector between the center of masses of the $(Z_T; e_2)$ and $(Z_P; e_1)$ in the exit channel of process (2.1).

The initial distorted wave can be expressed as a product of the initial bound state $\varphi_i(\vec{x}_1, \vec{x}_2)$ with the two Coulomb waves (one for the electronic and the other for the nuclear motion):

$$\chi_i^+ = N^+(\nu_P)\mathcal{N}^+(\nu)e^{i\vec{k}_i\cdot\vec{r}_i}\varphi_i(\vec{x}_1, \vec{x}_2)\,{}_1F_1(i\nu_P, 1, ivs_1 + i\vec{v}\cdot\vec{s}_1)\,{}_1F_1(-i\nu, 1, ik_i r_i - i\vec{k}_i\cdot\vec{r}_i). \tag{2.2}$$

Here, the symbol ${}_1F_1(a, b, c)$ denotes the conventional confluent hypergeometric function and normalization constants are defined by

$$N^+(\nu_P) = \Gamma(1 - i\nu_P)e^{\pi\nu_P/2},\ \mathcal{N}^{\pm}(\nu) = \Gamma(1 \pm i\nu)e^{-\pi\nu/2}, \tag{2.3}$$

where

$$\nu_P = \frac{Z_P}{v},\quad \nu = \frac{Z_P(Z_T - 1)}{v}. \tag{2.4}$$

Quantity $\vec{k}_i$ in eq. (2.2) represents the initial wave vector, whereas $\vec{v}$ is the vector of the incident velocity which is chosen along Z axes. The such treatment of the entrance channel is identical to that of the CDW-4B approximation [16,17].

The corresponding perturbation potential U_i which explicitly appears in the prior transition amplitude is given by [16,17]:

$$U_i = V_i - W_i \equiv Z_P \left(\frac{1}{R} - \frac{1}{s_2} \right) - \vec{\nabla}_{x_1} \ln \varphi_i(\vec{x}_1, \vec{x}_2) \cdot \vec{\nabla}_{s_1}, \tag{2.5}$$

where W_i is the distorting potential operator while V_i is the perturbation potential in the entrance channel:

$$V_i = \frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}. \tag{2.6}$$

It should be recalled that the distorted wave χ_i^+ possesses the proper asymptotic behaviour.

Using the distorting potential in the form

$$W_f = \frac{(Z_P - 1)(Z_T - 1)}{r_f}, \tag{2.7}$$

for the distorted wave χ_f^- in the exit channel we shall obtain

$$\chi_f^- = \mathcal{N}^+(\nu_f) \varphi_P(\vec{s}_1) \varphi_T(\vec{x}_2) e^{-i\vec{k}_f \cdot \vec{r}_f} {}_1F_1(i\nu_f, 1, -ik_f r_i - i\vec{k}_f \cdot \vec{r}_i), \tag{2.8}$$

where $\nu_f = (Z_P - 1)(Z_T - 1)/v$ and the final wave vector is labeled by $\vec{k}_f$. The bound state wave functions of the atomic systems (Z_P, e_1) and (Z_T, e_2) are denoted by $\varphi_P(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$, respectively. The distorted wave χ_f^- obeys the correct boundary condition.

The prior form of the transition amplitude, in the BDW model is [14]:

$$T_{if}^- = \langle \chi_f^- | U_i | \chi_i^+ \rangle, \tag{2.9}$$

or in explicit form this amplitude reads as:

$$T_{if}^-(\vec{\eta}) = N^+(\nu_P) \iiint d\vec{x}_1 d\vec{x}_2 d\vec{R} e^{i\vec{\alpha}\cdot\vec{s}_1 + i\vec{\beta}\cdot\vec{x}_1} \mathcal{L}^-(R) \varphi_P^*(\vec{s}_1) \varphi_T^*(\vec{x}_2) \left[Z_P \left(\frac{1}{R} - \frac{1}{s_2} \right) \right.$$
$$\left. \times \varphi_i(\vec{x}_1, \vec{x}_2) {}_1F_1(i\nu_P, 1, ivs_1 + i\vec{v}\cdot\vec{s}_1) - \vec{\nabla}_{x_1} \varphi_i(\vec{x}_1, \vec{x}_2) \cdot \vec{\nabla}_{s_1} {}_1F_1(i\nu_P, 1, ivs_1 + i\vec{v}\cdot\vec{s}_1) \right],$$

where the two momentum transfers s $\vec{\alpha}$ and $\vec{\beta}$ are defined as:

$$\vec{\alpha} = \vec{\eta} - v^- \hat{\vec{v}}, \ \vec{\beta} = -\vec{\eta} - v^+ \hat{\vec{v}}, \ v^\pm = \frac{v}{2} \pm \frac{\varepsilon_i - \varepsilon_f}{v}, \tag{2.10}$$

whereas $\vec{\eta}$ is the transverse component of the projectile momentum transfer and ε_i and ε_f represent the initial and final bound-state energies.

The function $\mathcal{L}^-(R)$ can be reduced as follows:

$$\begin{aligned}\mathcal{L}^-(R) &= (\mathcal{N}^+)^*(\nu_f)\mathcal{N}^+(\nu)\,{}_1F_1(-i\nu_f,1,ik_fr_i+i\vec{k}_f\cdot\vec{r}_i)\,{}_1F_1(-i\nu,1,ik_ir_i-i\vec{k}_i\cdot\vec{r}_i)\\ &\simeq (vR-\vec{v}\cdot\vec{R})^{iZ_P(Z_T-1)/v}(vR+\vec{v}\cdot\vec{R})^{i(Z_P-1)(Z_T-1)/v}\\ &= \rho^{2iZ_P(Z_T-1)/v}(vR+\vec{v}\cdot\vec{R})^{-i\xi},\end{aligned} \tag{2.11}$$

where $\xi=(Z_T-1)/v$. Here, $\vec{\rho}$ is the component of the vector of the internuclear distance perpendicular to the Z-axis ($\vec{R}=\vec{\rho}+\vec{Z}$). The factor $\rho^{2iZ_P(Z_T-1)/v}$ does not contribute to the total cross sections and may simply be omitted. It ought to be recalled that this factor does not disappear from the differential cross section.

The nine-dimensional integral for the matrix elements $T_{if}^-(\vec{\eta})$ can be analytically reduced in terms of *two*-dimensional real quadratures. The details of the computational procedures are not described here as they have been given in ref.[14].

Another one-channel distorted wave model can be formulated if we use for the initial state function:

$$\Phi_i=\varphi_i(\vec{x}_1,\vec{x}_2)e^{i\vec{k}_i\cdot\vec{r}_i}\mathcal{N}^+(\nu_i)\,{}_1F_1(-i\nu_i,1,ik_ir_i-i\vec{k}_i\cdot\vec{r}_i), \tag{2.12}$$

whereas the distorted wave χ_f^- in the exit channel is looked for in the form:

$$\begin{aligned}\chi_f^- &= \varphi_{PT}(\vec{s}_1,\vec{x}_2)e^{-i\vec{k}_f\cdot\vec{r}_f}\mathcal{N}^-(\nu)N^-(\nu_T)\\ &\quad\times{}_1F_1(-i\nu_T,1,-ivx_1-i\vec{v}\cdot\vec{x}_1)\,{}_1F_1(i\nu,1,-ik_fr_f+i\vec{k}_f\cdot\vec{r}_f),\end{aligned} \tag{2.13}$$

where $\varphi_{PT}(\vec{s}_1,\vec{x}_2)=\varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2)$, $\mathcal{N}^+(\nu_i)=e^{-\pi\nu_i/2}\Gamma(1+i\nu_i)$, $\nu_i=Z_P(Z_T-2)/v$, $N^-(\nu_T)=\Gamma(1+i\nu_T)e^{\pi\nu_T/2}$, $\nu_T=(Z_T-1)/v$, provided that distorted potential is chosen in the form

$$U_f=Z_P\left(\frac{1}{R}-\frac{1}{s_2}\right)-\left(\frac{1}{x_1}-\frac{1}{r_{12}}\right)-\vec{\nabla}_{s_1}\ln\varphi_{PT}(\vec{s}_1,\vec{x}_2)\cdot\vec{\nabla}_{s_1}. \tag{2.14}$$

The post form of the such model is given by:

$$T_{if}^+=\langle\chi_f^-|U_f|\Phi_i\rangle, \tag{2.15}$$

or the explicit expression for matrix elements reads as:

$$\begin{aligned}T_{if}^+ &= [N^-(\nu_T)]^*\iiint d\vec{x}_1d\vec{x}_2d\vec{R}e^{i\vec{k}_i\cdot\vec{r}_i+i\vec{k}_f\cdot\vec{r}_f}\varphi_i(\vec{x}_1,\vec{x}_2)\mathcal{L}^+(R)\\ &\times\left\{{}_1F_1(i\nu_T,1,ivx_1+i\vec{v}\cdot\vec{x}_1)\left[Z_P\left(\frac{1}{R}-\frac{1}{s_2}\right)-\left(\frac{1}{x_1}-\frac{1}{r_{12}}\right)\right]\varphi_P^*(\vec{s}_1)\varphi_T^*(\vec{x}_2)-\right.\\ &\left.-\varphi_T^*(\vec{x}_2)\vec{\nabla}_{s_1}\varphi_P^*(\vec{s}_1)\cdot\vec{\nabla}_{x_1}{}_1F_1(i\nu_T,1,ivx_1+i\vec{v}\cdot\vec{x}_1)\right\},\end{aligned} \tag{2.16}$$

where the function $\mathcal{L}^+(R)$ can be reduced as

$$\begin{aligned}\mathcal{L}^+(R) &= N^+(\nu_i)\,{}_1F_1(-i\nu_i, 1, ik_ir_i - i\vec{k}_i\cdot\vec{r}_i)[N^-(\nu)]^*\,{}_1F_1(-i\nu, 1, ik_fr_f - i\vec{k}_f\cdot\vec{r}_f)\\ &\simeq (k_ir_i - \vec{k}_i\cdot\vec{r}_i)^{i\nu_i}(k_fr_f - \vec{k}_f\cdot\vec{r}_f)^{i\nu} \simeq \mu_i^{i\nu_i}\mu_f^{i\nu}(vR - \vec{v}\cdot\vec{R})^{i\nu_i}(vR + \vec{v}\cdot\vec{R})^{i\nu}\\ &= \mu_i^{i\nu_i}\mu_f^{i\nu}[v^2(R^2 - Z^2)]^{i\nu_i}(vR + \vec{v}\cdot\vec{R})^{-i\xi} = \mu_i^{i\nu_i}\mu_f^{i\nu}(\rho v)^{2i\nu_i}(vR + \vec{v}\cdot\vec{R})^{-i\xi}.\end{aligned}$$

where now $\xi = \nu_i - \nu = -Z_P/v$. Evaluation of the post form of the transition amplitude is more difficult only from numerical point of view. Namely, the term $1/r_{12}$ in the eq. (2.17) requires an additional three-dimensional integral which must be treated numerically. Therefore the matrix elements T_{if}^+ can be analytically reduced to a five-dimensional quadrature. For this reason in the present work, numerical computations are carried out only for prior form.

3. Results and discussions

The differential cross section is defined by the relation (see for example review article [21]):

$$\frac{dQ_{if}}{d\Omega} = \frac{\mu_i\mu_f}{4\pi^2}\,|T_{if}(\vec{\eta})|^2 \quad \left(\frac{a_0^2}{sr}\right).$$

the quantity μ_i is the reduced mass of the projectile and the target and μ_f is reduced mass of the two aggregates $(Z_P; e_1)$ and $(Z_T; e_2)$ in the exit channel. The scattering angle θ is defined by the relation $\eta = 2\mu_{PT}v\sin(\theta/2)$, where μ_{PT} is the reduced mass of the projectile and target nucleus. Calculation of the angular distributions $dQ_{if}/d\Omega$ becomes particularly convenient in the BDW approximation when proton is used as a projectile i.e. $Z_P = 1$. This is because the products of the logarithmic Coulomb phase factors from the function $\mathcal{L}^-(R)$ defined by eq. (2.11) will be reduced to the single term $(vR - \vec{v}\cdot\vec{R})^{i\xi}$. Hence, a trivial modification of the sign of the parameter ξ, as well as of the sign of the term $\vec{v}\cdot\vec{R}$, will enable us to obtain both differential [with factor $(vR - \vec{v}\cdot\vec{R})^{i\xi}$] and total cross sections [with factor $(vR + \vec{v}\cdot\vec{R})^{-i\xi}$] from the same algorithm associated with the BDW method. It should be noted that the computation of the differential cross section in the four-body CDW method becomes a much more laborious task, involving highly oscillating Bessel functions and evaluation of the transition amplitude $\mathcal{A}_{if}(\vec{\rho})$ by means of the Fourier transform $\mathcal{A}_{if}(\vec{\rho}) = (2\pi)^{-1}\int d\vec{\kappa}e^{i\vec{\kappa}\cdot\vec{\rho}}T_{if}^{CDW}(\vec{\kappa})$.

As an illustration, BDW approximation is utilized to compute differential cross sections for reaction

$$p + He \longrightarrow H + He^+.$$

The present computations are carried out by using the uncorrelated one parameter wave function for the initial bound state of the target: $\varphi_i(\vec{x}_1, \vec{x}_2) = (\gamma^3/\pi)e^{-\gamma(x_1+x_2)}$,

where γ is the effective charge $\gamma = Z_T - 5/16$. In figure 1 theoretical differential cross sections at $500\,keV$ are plotted (full line) together with recent experimental data of Mergel *et al* [5]. As can be seen, the the computed DCS are in good agreement with the experimental measurements. In this work we shall evaluate the role of the term $V(R, s_2) = Z_P(1/R - 1/s_2)$ in the considered reaction. Namely, when we neglect this term from eq. (2.5), we obtain results for DCS which are displayed in Figure 1 by dashed curve. As can be seen, the contribution from the potential $V(R, s_2)$ in the DCS is negligible at small scattering angles. This potential is significant at larger scattering angles. However, this difference between theories with and without the potential $V(R, s_2)$ at larger scattering angles is not so strongly apparent in the total cross sections, which are predominantly determined by collisions near the narrow forward direction.

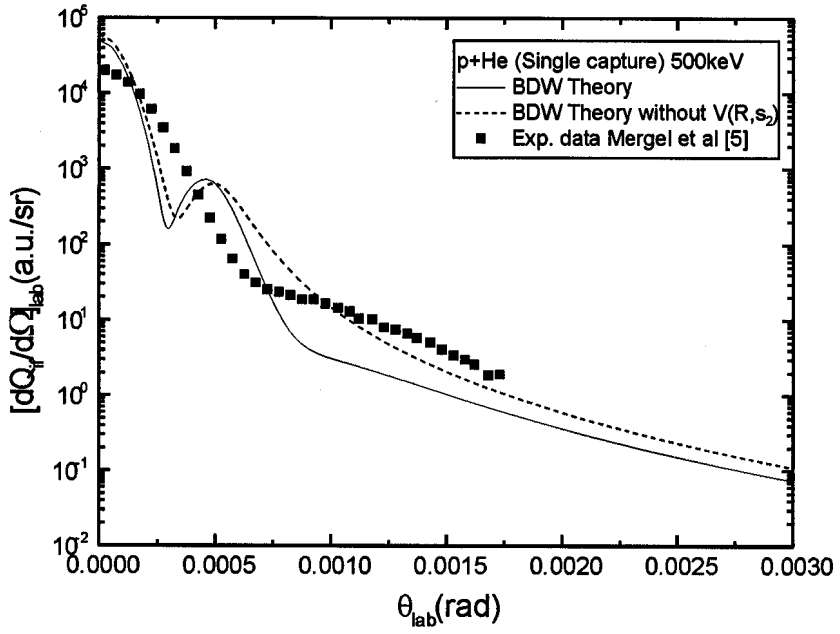

Figure 1. The differential cross sections $dQ_{if}/d\Omega(a.u./sr)$ as a function of scattering angle $\theta(rad)$ for $500\,keV$ proton impact. Both cross sections and scattering angle are in the laboratory system. Full curve: our BDW results. Dashed curve: our BDW results obtained without potential $V(R, s_2) = Z_P(1/R - 1/s_2)$. Experimental data: ■ Mergel *et al* [5].

The theoretical results include capture only in the ground state, while the contribution from the excited states is accounted for by the factor 1.202 which addition-

ally multiplies the cross sections according to Oppenheimer scaling law. It should be emphasized that DCS are obtained by BDW method via two-dimensional real quadratures. This is a great advantage in the application of the theory because it allows for a very fast numerical calculation of the differential cross section.

4. Conclusions

We have investigated single electron capture in $p+He$ collisions by means BDW approximation. The computations of the differential cross sections are performed at $500\,keV$. A comparison with experimental data is made and a good agreement is found. We have also studied the role of the potential $V(R, s_2)$. It should be recalled that DCS provides the most stringent test for theory, since any integration over observables often masks important characteristics of the process.

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ČETVOROČESTIČNE JEDNOKANALNE TEORIJE IZOBLIČENIH TALASA ZA ZAHVAT ELEKTRONA

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Dve verzije modela izobličenih talasa su formulisane u okviru četvoročestične teorije sudara. Kao ilustracija, BDW aproksimacija je primenjena za izračunavanje diferencijalnih preseka za jednostruki zahvat elektrona u procesu sudara protona sa heliumom na energiji od 500 keV. Dobijeni rezultati su u dobrom slaganju sa eksperimentalnim podacima.