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EXCITATION OF THE HYDROGEN ATOM FROM THE METASTABLE 2s-STATE BY ELECTRON IMPACT

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Excitation of hydrogen atom from its metastable 2s-state to ns ($n = 3, 4, 5, 6$) and np ($n = 3$) states by electron impact has been investigated by employing a distorted-wave method, in the framework of the two-potential formulation. Contribution of exchange has been included by antisymmetrising the total wave function of the system. The differential cross-sections are reported at intermediate energies. Theoretical findings for 2s-5s and 2s-6s transitions have not been reported earlier.

1. *Introduction*

Recently, interest bas been focussed on the excitation of atoms from their metastable states. This is due to the applications in astrophysics, laser physics, gaseous discharge and plasma physics. Apart from that, these investigations reveal the dynamics of collision processes.

Excitation of atoms by electron impact has been reviewed by Bransden and McDowell [1,2]. Calculations of excitation cross-sections from metastable states have been carried out mainly on electron-helium scattering. Kim and Inokuti [3] have employed the first-order Born approximation to investigate e^--He scattering. Similar calculation has also been carried out by Flannery et al. [4] and Ton-That et al. [5]. Apart from these, investigations have been carried out by employing the multichannel eikonal approximation (Flannery and McCan [6]) and the Glauber approximation (Chen and Khayrallah [7]). In recent past convergent close coupling

[8] and IERM [9] techniques have been used for investigating excitation processes in case of hydrogen. Sharma et al. [10] employed the distorted-wave method to obtain differential cross–sections for excitation from metastable state of hydrogen and helium. The distorted–wave employed by them is the Coulomb wave function with screened nuclear charge, adjusted following the method suggested by Junker [11]. Without antisymmetrizing the total wave function of the system, the effect of exchange is included using Ochkur [12] approximation.

Recently, Verma and Srivastava [13] have reported cross-sections for electron impact excitation of hydrogen from metastable 2s state to 3s and 3p states in distorted-wave approximation. They have taken distortion potential (static potential of the final state of the target and the semiclassical exchange potential of Furness and McCarthy [14]) to be the same for both channels.

In the present study, we investigate the excitation of H-atom from its 2s metastable state by electron impact. The method employs the first-order distorted-wave Born approximation (DWBAI) based on the two-potential approach. The present form of DWBAI is similar to that of Madison and Shelton [15]. In our investigation, both the incident and the scattered electrons are represented by distorted-waves which have been evaluated using an arbitrary potential. However, the choice of arbitrary potential (here it is taken as the static potential in the initial channel) is not unique. The effect of exchange has been taken by antisymmetrising the total wave function of the system. We report differential cross-sections for the 2s-ns ($n = 3, 4, 5, 6$) and 2s-3p excitations of the hydrogen atom at medium energies.

2. Theory

The total Hamiltonian for the electron-hydrogen system is expressed as:

$$H = H_0 + H_{at} + V, \tag{1}$$

where H_0 is the free particle Hamiltonian and H_{at} is that of the target atom. The interaction potential is expressed as:

$$V = -\frac{z}{x} + \frac{1}{|\vec{x} - \vec{r}|}, \tag{2}$$

In the framework of two-potential approach, the exact T-matrix from the initial state $|n_i>$ with momentum $\mathbf{k}_i$ to the final state $< n_f|$ with momentum $\mathbf{k}_f$ is given by

$$T_{if} = < \chi_f^- n_f | V - U_f | A \psi_i^+ >< \chi_f^- n_f | U_f | \beta_i n_i >, \tag{3}$$

where β_i is the initial-state plane wave (eigenfunction for an isolated projectile). Ψ_i^+ is the initial state full scattering wave function which is solution of Schrődinger equation:

$$(H - E)\ \psi_i^+ = 0. \tag{4}$$

A used in Eq. (3) is the antisymmetric operator.

U_f is chosen as a spherically symmetric arbitrary distorting potential that satisfies the required boundary conditions. The potential U_f is also used to evaluate x_f^-, i.e.,

$$(H_0 + U_f - E_f)\ \chi_f^- = 0, \tag{5}$$

The full scattering wave function for the initial state can be expanded in terms of the full Green's function G^+ as

$$|\psi_i^+> = |n_i\chi_i^+> + G^+(V - U_i)|n_i\chi_i^+>, \tag{6}$$

where χ_i^+ satisfies the Schrődinger equation

$$(H_0 + U_i - E_i)\ \chi_i^+ = 0. \tag{7}$$

Here U_i is also an arbitrarily chosen spherically symmetric distorting potential which satisfies the asymptotic condition. Using Eq. (6) and the expansion of Green's function, the first–order distorted–wave transition matrix takes the form

$$T_{if}^s = f + (-1)^s g$$

where

$$f = <\chi_f^- n_f|\frac{1}{|\vec{x} - \vec{r}|}|n_i\chi_i^+>$$

$$g = <\chi_f^- n_f|\frac{1}{|\vec{x} - \vec{r}|}|n_i\chi_i^+> - <\chi_f^-|U_f|n_i><n_f|\chi_i^+> .$$

In the exchange amplitude, the contribution of overlap integral is expected to be small. According to this consideration one may neglect the second term of the exchange amplitude.

We evaluate the direct and the exchange amplitudes by using partial wave analysis. Details of the calculations are provided in Appendix.

3. *Numerical methods*

$\chi_f^-(\vec{k}_f, \vec{r})$ and $\chi_i^+(\vec{k}_i, \vec{r})$ have been evaluated following the Numerov method and the total wave function is normalised accordingly. Radial integration has been carried out up to 120 atomic units with the step size of 0.01. It has been found that the real part of the phase shift for 2s $\rightarrow$ ns transition is absolutely convergent with respect to the step size. For the case of s $\rightarrow$ s transition, we have performed the calculation up to the angular momentum $l = 60$, whereas for the case of s $\rightarrow$ p transition, summation over angular momentum has been performed up to $l = 99$ at the the highest energy considered. Higher partial wave contributions are substituted by the Born term whenever required. We evaluate the radial integral by breaking the length in accordance with the zeros of the Bessel function and 16 point Gaussian quadrature was employed for each integral.

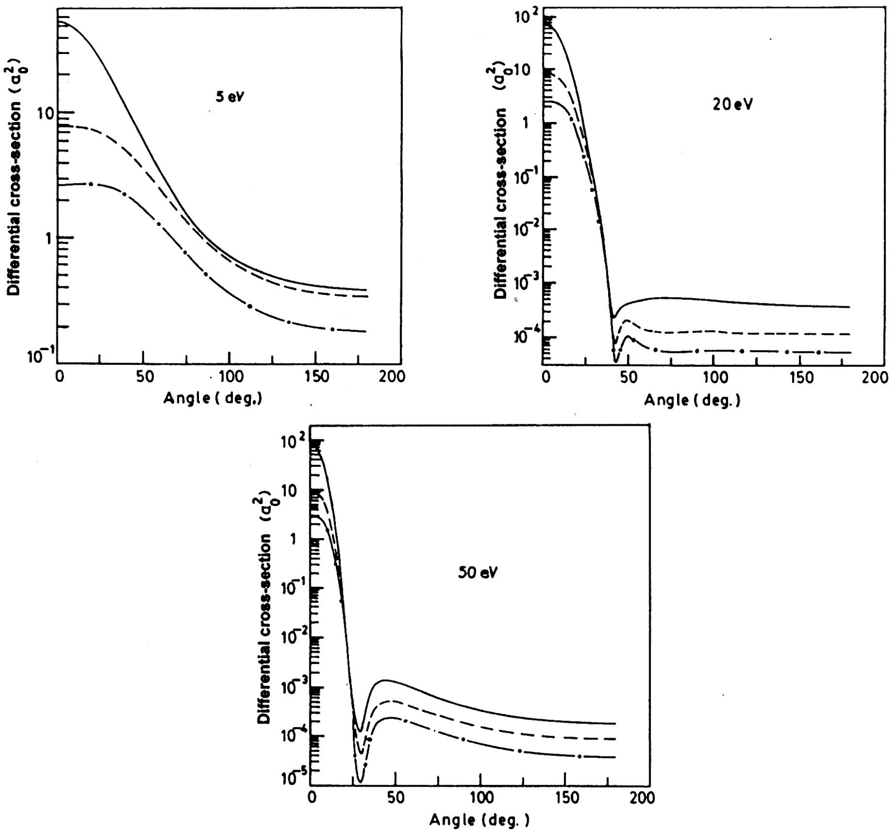

Fig. 1. Differential cross-sections for electron impact excitation of hydrogen atom: — · — · — for 2s → 3s, – – – – for 2s → 4s and ———— for 2s → 5s: a) at 5 eV, b) at 20 eV and c) at 50 eV.

4. Results and discussion

We report the differential cross-setions for (2s → 3s), (2s → 4s),(2s → 5s), (2s → 6s) and (2s → 3p) transitions in e^-–H scattering. In Fig. 1, we have plotted the differential cross-sections for the 2s → ns ($n = 3, 4, 5$) transitions at three different energies. The features for all transitions involving the 3s, 4s, 5s states have been found to be the same. The 2s → 6s transition also shows the same features (not shown in figure, refer to Table 4).

First, we discuss the case of s → s transitions. At low energy, say 5 eV, no minimum in the angular distributions has been noticed for transitions to 3s, 4s, 5s states (Fig. 1a). With the enhancement of energy (to 20 eV), we find a minimum

(Fig. 1b). This minimum turns out to be deeper when the energy is increased to 50 eV (Fig. 1c) and above. In our earlier communication (Jha et al. [16]), this feature has also been noticed.

TABLE 1.

Differential cross–sections for 2s → 3s excitation of hydrogen atom by electron impact (distorted–wave results with exchange) in units of a_0^2.

Angle	Energy (eV)				
(deg)	10.0	30.0	80.0	100.0	150.0
0.0	6.89E+01	8.73E+01	9.41E+01	9.49E+01	9.52E+01
5.0	6.30E+01	6.45E+01	4.11E+01	3.37E+01	2.04E+01
10.0	4.83E+01	2.64E+01	3.80E+00	1.74E+00	2.43E-01
15.0	3.13E+01	6.29E+00	7.60E-02	9.64E-03	1.33E-04
20.0	1.73E+01	9.11E-01	4.38E-05	8.83E-06	1.53E-04
25.0	8.37E+00	7.65E-02	1.18E-05	3.95E-04	6.98E-04
30.0	3.61E+00	3.08E-03	7.42E-04	7.13E-04	3.69E-04
35.0	1.41E+00	1.37E-04	8.88E-04	6.13E-04	1.55E-04
40.0	5.15E-01	2.42E-04	7.39E-04	4.25E-04	1.29E-04
50.0	5.90E-02	1.20E-03	4.00E-04	1.87E-04	2.48E-05
60.0	7.05E-03	1.52E-03	2.26E-04	9.37E-05	2.26E-05
80.0	7.87E-04	1.30E-03	9.78E-05	3.64E-05	4.86E-06
100.0	6.24E-04	1.00E-03	5.72E-05	2.02E-05	1.61E-06
120.0	4.21E-04	8.11E-04	4.05E-05	1.40E-05	1.57E-06
140.0	3.46E-04	6.93E-04	3.24E-05	1.11E-05	1.06E-06
160.0	3.05E-04	6.38E-04	2.85E-05	9.83E-06	2.09E-07
180.0	2.93E-04	6.20E-04	2.76E-05	8.81E-06	1.34E-07

On the other hand, FBA predicts two zeros in the angular distribution of inelastic scattering. In our opinion, this is due to the nodal properties of the wave function of the hydrogen atom. Our distorted-wave result, instead, provides only single minimum at intermediate energies. We understand that the effect of exchange and the distorted wave might have cancelled the nodal properties of the wave function employed.

The excitation of hydrogen atom from its 2s-metastable state has also been investigated by Sharma et al. using three models (Born-Ochkur, distorted wave with Ochkur having two different screening parameters). Their distorted-wave results are very sensitive to the effective parameter δ and they differ dramatically from their Born-Ochkur results. Their distorted-wave differential cross-section (with $\delta = 1$) near the forward direction $\theta < 2^\circ$ is nearly half of their Born-Ochkur results. On the other hand, their differential cross-section near the backward direction is nearly 60 fold higher than their Born-Ochkur results. Effect of Coulomb wave in the final channel might be responsible for this. Considering all these facts, we compare the present results at 20 eV and 50 eV with those of Sharma et al. (Born-Ochkur) and FBA for the case of 2s → 3s transition (see Figs. 2a and b). Results of Sharma et al.

show a deep minimum at all energies. It may be mentioned that their distorted-wave results with exchange (Ochkur type) do not show any minimum at all. Up to the

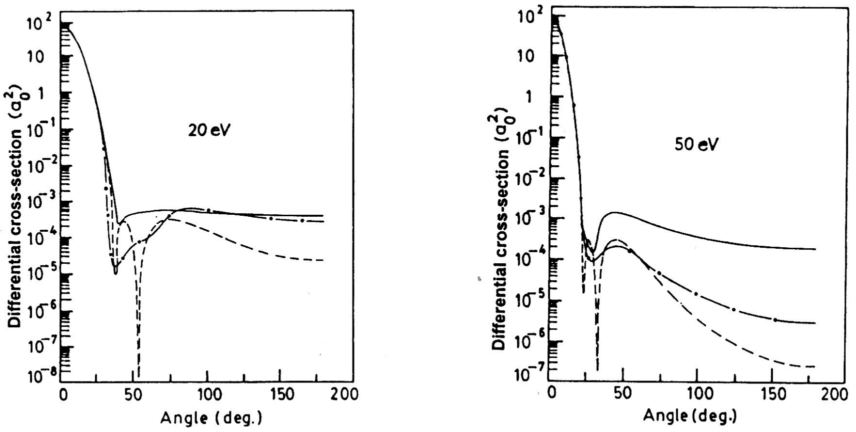

Fig. 2. Diff. cross–sections for electron–impact 2s → 3s excitation of hydrogen atom:
————— present results, — · — · — Born-Ochkur results of Sharma et al. [8] and — — — — Born results: a) at 20 eV and b) at 50 eV.

TABLE 2.
Differential cross-sections for 2s → 4s excitation of hydrogen atom by electron impact (distorted-wave results with exchange) in units of a_0^2.

Angle (deg)	Energy (eV) 10.0	30.0	80.0	100.0	150.0
0.0	7.28E+00	9.37E+00	1.02E+01	1.03E+01	1.08E+01
5.0	7.11E+00	8.50E+00	7.35E+00	6.66E+00	4.91E+00
10.0	6.55E+00	5.57E+00	1.44E+00	7.49E-01	1.24E-01
15.0	5.51E+00	2.13E+00	4.81E-02	8.28E-03	9.02E-06
20.0	4.10E+00	4.33E-01	4.80E-05	1.32E-05	9.23E-05
25.0	2.63E+00	5.97E-02	2.79E-05	8.94E-05	1.24E-04
30.0	1.46E+00	2.82E-03	2.12E-04	2.85E-04	1.46E-04
35.0	7.10E-01	3.96E-05	3.31E-04	2.39E-04	1.20E-04
40.0	3.14E-01	4.46E-05	2.93E-04	1.61E-04	3.35E-05
50.0	5.24E-02	3.32E-04	1.68E-04	7.63E-05	2.41E-05
60.0	7.92E-03	5.65E-04	9.55E-05	4.05E-05	3.38E-06
80.0	6.41E-04	5.25E-04	4.05E-05	1.58E-05	2.29E-06
100.0	3.34E-04	4.29E-04	2.30E-05	8.99E-06	2.16E-06
120.0	2.76E-04	3.59E-04	1.59E-05	5.95E-06	9.40E-07
140.0	2.00E-04	3.21E-04	1.25E-05	4.74E-06	3.10E-07
160.0	1.73E-04	2.92E-04	1.13E-05	4.01E-06	2.69E-07
180.0	1.69E-04	2.84E-04	1.06E-05	3.71E-06	2.20E-07

scattering angle 30°, the present results are in close agreement with those of Sharma et al. and FBA at 20 eV. Present results differ qualitatively from others near the region of minimum (35°-60°). Beyond the scattering angle 60°, FBA results differ quantitatively from the present results, FBA results being appreciably lower. It may be mentioned that beyond 75°, the Born-Ochkur results of Sharma et al. are in good agreement with the present calculations. Differential cros-sections including exchange at selected energies are provided in Tables 1–4.

Table 5 displays the present differential cross-sections and those of Verma and Srivastava (V&S) for the 2s $\rightarrow$ 3p transition. They have reported results at impact energies 10 eV and 20 eV only. In case of 2s $\rightarrow$ 3s transition, there is considerable discrepancy between the two sets of calculations, the results of V&S being about 2–3 orders of magnitude higher than the present predictions at large scattering angles. Hence, they are not shown here. The corresponding cross-sections of two sets of calculations for 2s $\rightarrow$ 3p transition differ within a factor of 3 from each other, even at large scattering angles.

In the present distorted-wave approach, the distortion potential has been taken as static potential of the initial state and the exchange has been included by antisymmetrizing the total wave functions of the system. V&S have expressed the distortion potential as the sum of static potential and the semiclassical exchange potential, both corresponding to the final state of the target. The differences between the two sets of results may be attributed to the fact that results are sensitive to the form of the potential used in the calculations.

TABLE 3.
Differential cross-sections for 2s $\rightarrow$ 5s excitation of hydrogen atom by electron impact (distorted-wave results with exchange) in units of a_0^2.

Angle	Energy (eV)				
(deg)	10.0	30.0	80.0	100.0	150.0
0.0	2.20E+00	2.77E+00	3.03E+00	3.06E+00	3.20E+00
5.0	2.20E+00	2.69E+00	2.59E+00	2.42E+00	1.93E+00
10.0	2.14E+00	2.06E+00	6.78E-01	3.76E-01	7.17E-02
15.0	1.96E+00	9.42E-01	2.87E-02	5.31E-03	1.20E-05
20.0	1.60E+00	2.28E-01	5.65E-05	6.82E-06	3.27E-05
25.0	1.15E+00	2.95E-02	8.39E-06	3.86E-05	6.19E-05
30.0	7.12E-01	1.84E-03	9.91E-05	1.32E-04	7.49E-05
35.0	3.88E-01	2.20E-05	1.64E-04	1.18E-04	5.87E-05
40.0	1.91E-01	7.01E-06	1.47E-04	8.25E-05	1.72E-05
50.0	3.90E-02	1.21E-04	8.66E-05	3.85E-05	1.19E-05
60.0	7.71E-03	2.33E-04	5.01E-05	2.02E-05	1.87E-06
80.0	9.89E-04	2.26E-04	2.20E-05	7.93E-06	1.21E-06
100.0	6.05e-04	1.83E-04	1.29E-05	4.46E-06	1.21E-06
120.0	5.12E-04	1.51E-04	9.11E-06	2.97E-06	4.69E-07
140.0	4.35E-04	1.33E-04	7.34E-06	2.36E-06	1.65E-07
160.0	3.98E-04	1.21E-04	6.55E-06	2.02E-06	1.48E-07
180.0	3.88E-04	1.17E-04	6.23E-06	1.18E-06	1.45E-07

TABLE 4.
Differential cross–sections for 2s → 6s excitation of hydrogen atom by electron impact (distorted–wave results with exchange) in units of a_0^2.

Angle (deg)	Energy (eV) 10.0	30.0	80.0	100.0	150.0
0.0	9.34E-01	1.21E+00	1.49E+00	1.62E+00	1.82E+00
5.0	9.32E-01	1.20E+00	1.18E+00	1.09E+00	8.57E-01
10.0	9.29E-01	9.91E-01	3.76E-01	2.27E-01	5.74E-02
15.0	8.64E-01	4.86E-01	1.68E-02	2.58E-03	1.31E-04
20.0	7.20E-01	1.26E-01	2.39E-05	2.27E-06	5.62E-05
25.0	5.22E-01	1.70E-02	2.04E-05	5.51E-05	3.82E-05
30.0	3.27E-01	1.04E-03	7.40E-06	1.17E-05	2.98E-05
35.0	1.79E-01	1.33E-05	1.56E-04	1.43E-04	2.58E-05
40.0	8.72E-02	2.03E-06	2.69E-05	8.74E-06	2.27E-05
50.0	1.69E-02	5.08E-05	3.02E-05	1.19E-05	1.28E-06
60.0	3.50E-02	8.57E-05	3.08E-05	1.17E-05	2.33E-06
80.0	5.75E-04	7.17E-05	7.91E-06	3.65E-06	7.90E-07
100.0	3.90E-04	5.27E-05	1.86E-06	7.92E-07	9.92E-08
120.0	3.17E-04	4.12E-05	1.83E-06	7.87E-07	3.69E-08
140.0	2.70E-04	3.45E-05	1.58E-06	6.19E-07	2.98E-08
160.0	2.49E-04	3.12E-05	1.43E-06	5.69E-07	2.96E-08
180.0	2.41E-04	3.03E-05	1.41E-06	5.55E-07	2.22E-08

TABLE 5.
Differential cross–sections for 2s → 3p excitation of hydrogen atom by electron impact in units of a_0^2.

Angle	E=10 eV		E=20 eV	
(deg)	Present	V & S	Present	V & S
0.0	0.19E+04	0.14E+04	0.39E+04	0.30E+04
10.0	0.16E+03	0.20E+03	0.39E+03	0.20E+03
20.0	0.35E+02	0.18E+02	0.56E+01	0.10E+02
30.0	0.91E+01	0.71E+01	0.62E+00	0.13E+01
40.0	0.16E+01	0.30E+01	0.11E+00	0.25E+00
50.0	0.62E+00	0.10E+01	0.95E-01	0.23E+00
60.0	0.50E+00	0.81E+00	0.49E-01	0.10E+00
70.0	0.38E+00	0.50E+00	0.21E-01	0.50E-01
80.0	0.15E+00	0.25E+00	0.11E-01	0.25E-01
90.0	0.11E+00	0.20E+00	0.79E-02	0.16E-01
100.0	0.71E-01	0.13E+00	0.70E-02	0.10E-01
120.0	0.38E-01	0.70E-01	0.24E-02	0.50E-02
140.0	0.35E-01	0.70E-01	0.19E-02	0.40E-02
160.0	0.34E-01	0.80E-01	0.14E-02	0.30E-02
180.0	0.32E-01	0.90E-01	0.11E-02	0.25E-02

From a close inspection of the results, we find that in the case of 2s $\to$ 3p transitions, our DCS are in satisfactory agreement with those of V & S. For this excitation, their distorted-wave electron and positron results differ appreciably from each other as expected. On the other hand, their electron results differ from the present calculations by a large factor in the case of 2s-3s transition. At the same time, it is surprising that their distorted-wave electron and positron results are almost identical in this case. More elaborate theoretical studies are required to resolve these discrepancies and understand the dynamics of the system properly.

Appendix

Distorted-wave direct scattering amplitude from the initial state 2s with momentum $\mathbf{k}_i$ to the final state $n,' l,' m'$ with final momentum $\mathbf{k}_f$ is given by:

$$f = -\frac{1}{2\pi} \int \chi_f^{-*}(\vec{k}_f, \vec{x}) \; \Phi^*_{n'l'm'}(\vec{r}) \; \frac{1}{|\vec{x}-\vec{r}|} \; \Phi_{2s}(\vec{r})\chi_i^+(\vec{k}_i, \vec{x}) \mathrm{d}\vec{r} \; \mathrm{d}\vec{x}.$$

The continuum wave functions χ_f^- and χ_i^+ are expanded in terms of spherical harmonics as:

$$\chi_i^+ = \frac{4\pi}{\sqrt{k_i}x} \sum_{l_i, m_i} (\mathrm{i})^{l_i} \chi_{l_i}(k_i, x) Y^*_{l_i m_i}(\hat{\vec{x}}) Y_{l_i m_i}(\hat{\vec{k}}_i),$$

$$\chi_f^- = \frac{4\pi}{\sqrt{k_f}x} \sum_{l_f, m_f} (\mathrm{i})^{-l_f} \chi_{l_f}(k_f, x) Y^*_{l_f m_f}(\hat{\vec{x}}) Y_{l_f m_f}(\hat{\vec{k}}_f).$$

Taking k_i along the polar axis, and performing the integration over the angular parts of $\mathrm{d}\hat{\vec{r}}\; \mathrm{d}\hat{\vec{x}}$, we get,

$$f = \frac{8\pi}{\sqrt{k_i k_f}} \sum_{l_i} \sum_{l_f} (\mathrm{i})^{l_i - l_f} \left(\frac{(2l_f+1)(2l'+1)}{4\pi} \right)^{1/2} \begin{pmatrix} l_f & l' & l_i \\ -m' & m' & 0 \end{pmatrix}$$

$$\begin{pmatrix} l_f & l' & l_i \\ 0 & 0 & 0 \end{pmatrix} Y_{l_f, -m'}(\hat{\vec{k}}_f) \int \chi_{l_i}(k_i, x) \chi_{l_f}(k_f, x) R_{n'l'}(x) \mathrm{d}x,$$

where

$$R_{n'l'}(x) = \int P_{n'l'}(r) P_{2s}(r) A_{l'}(r \neq x) \mathrm{d}r.$$

P's are radial wave functions of hydrogen multiplied by r, and $A_l' = r_<^{l'}/r_>^{l'+1}$.

When the exchange effect is taken into account, the scattering amplitude reads:

$$g = -\frac{1}{2\pi} \int \chi_f^{-*}(\vec{k}_f, \vec{r}) \; \Phi^*_{n'l'm'}(\vec{x}) \; \frac{1}{|\vec{x}-\vec{r}|} \; \Phi_{2s}(\vec{r})\chi_i^+(\vec{k}_i, \vec{x}) \; \mathrm{d}\vec{r}\mathrm{d}\vec{x}.$$

Proceeding in the same way, we get,

$$g = \frac{-32\pi^2}{\sqrt{4\pi k_i k_f}} \sum_{l_i} \sum_L (\mathrm{i})^{l_i - L} \left(\frac{(2L+1)(2l'+1)}{4\pi} \right)^{1/2} \begin{pmatrix} L & l' & l_i \\ -m' & m' & 0 \end{pmatrix}$$

$$\begin{pmatrix} L & l' & l_i \\ 0 & 0 & 0 \end{pmatrix} Y_{L,-m'}(\hat{\vec{k}}_f) \int \chi_{l_i}(k_i, x) P_{n'l'}(x) \mathrm{d}x \int \chi_L(k_f, r) P_{2s}(r) A_L(r \neq x) \mathrm{d}\vec{r}.$$

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UZBUDA VODIKA S METASTABILNOG 2s–STANJA UDAROM ELEKTRONA

Istražuje se uzbuda vodikovog atoma iz 2s–stanja u ns ($n = 3, 4, 5, 6$) i np ($n = 3$) stanje upotrebom distordiranih valova i na osnovi dvopotencijalne funkcije. Daju se diferencijalni udarni presjeci za srednje energije elektrona.