Excitation of hydrogenlike ions from ground state to arbitrary *p* state by electron impact

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We have formulated a generalized method for the evaluation of the cross sections for $1s$-np excitation of hydrogenlike ions by electron impact both in Coulomb-Born and Coulomb-Born-Oppenheimer (CBO) approximations. In this formulation we have replaced the associated Laguerre polynomial for the final-state wave function by an integral representation. The main advantage of our method is that the higher-order parametric differentiations usually adopted in order to obtain the amplitudes for the higher values of the principal quantum number n are avoided by one-dimensional integration. To our knowledge, this is the first attempt to calculate the electron-ion excitation cross section in the CBO approximation for an arbitrary p state without any recourse to partial-wave analysis. We have also calculated asymptotic scaled cross sections for the limit $n \to \infty$ at different energies. The direct-excitation results are in good agreement with the existing theoretical findings of Tully for different n values in the intermediate- and high-energy regions.

I. INTRODUCTION

The study of electron-impact excitation of one-electron ions is considered to be of great interest because of its wide application in various astrophysical and plasma phenomena. Apart from the experimental studies of Dolder and Peart[1] and Dashchenko *et al.*,[2] there are a number of theoretical works[3–22] on the electron-impact excitation of hydrogenlike ions in different approaches. The early theoretical attempts by Burgess *et al.*,[3] and by Tully[4] to investigate such excitation processes for some low-lying states in the Coulomb-Born-Oppenheimer (CBO) and Coulomb-Born (CB) approximations were based on the partial-wave expansion. However, the partial-wave treatment is not suitable in many cases owing to the requirement of a large number of partial waves. Mitra and Sil[9,13] first suggested a new method of evaluation for the $1s$-$2s$ and $1s$-$2p$ excitation cross sections of hydrogenlike ions in both CB and CBO approximations without any recourse to partial-wave analysis. The matrix element appearing in the $1s$-$2p$ CB amplitude in their work[13] required a one-dimensional integration to be carried out numerically, while in a contemporary work, Sung Dahm Oh *et al.*[15] presented a closed-form expression for the same matrix element. In a later development,[14,17] the earlier method of Mitra and Sil[9] was suitably generalized to include the excitation of any arbitrary s state in an easily computable way.

In this paper, we have presented a generalized method taking account of the exchange effect for the calculation of the cross section of electron-impact excitation of hydrogenlike ions to an arbitrary p state including the asymptotic limit of the principal quantum number n. For the direct case we have based our extension on the closed-form expression of $1s$-$2p$ amplitude of Sung Dahm Oh *et al.*,[15] while for the exchange part we have followed the earlier work of Sinha and Sil[17] for $1s \to ns$ amplitude.

II. THEORY

A. Direct amplitude

The expression for the direct amplitude for the transition from $1s$ to np state of hydrogenlike ions under electron impact in the CB approximation is given by

$$T_{1s-np} = -\frac{1}{2\pi} \int \int \phi_{np_{x,z}}(\vec{r}_2)\psi^{(-)*}_{\vec{K}_f}(\vec{r}_1)\frac{1}{r_{12}}\phi_{1s}(\vec{r}_2)\psi^{(+)}_{\vec{K}_i}(\vec{r}_1)d\vec{r}_1 d\vec{r}_2 , \quad (1)$$

where

$$\psi^{(+)}_{\vec{K}_i}(\vec{r}_1)=\exp\left[\pi\frac{Z-1}{2K_i}\right]\Gamma(1-a)e^{i\vec{K}_i\cdot\vec{r}_1}{}_1F_1(a,1;i(K_ir_1-\vec{K}_i\cdot\vec{r}_1)) ,$$
$$\psi^{(-)}_{\vec{K}_f}(\vec{r}_1)=\exp\left[\pi\frac{Z-1}{2K_f}\right]\Gamma(1+b)e^{i\vec{K}_f\cdot\vec{r}_1}{}_1F_1(-b,1;-i(K_fr_1+\vec{K}_f\cdot\vec{r}_1)) \qquad (1')$$

with $a=i(Z-1)/K_i$, $b=i(Z-1)/K_f$, and Z is the nuclear charge.

The ground-state hydrogenlike wave function ϕ_{1s} and the generalized final-state wave function $\phi_{np_{x,z}}$ are given by

$$\phi_{1s}(\vec{r}_2)=N_{1s}e^{-\lambda_1r_2},\quad N_{1s}=z^{3/2}/\sqrt{\pi},\quad \lambda_1=Z \qquad (1'')$$

$$\phi_{np_{x,z}}(\vec{r}_2)=N_{np}r_{2x,z}e^{-\lambda_nr_2}L^3_{n+1}(2\lambda_nr_2),\quad N_{np}=\frac{2\lambda_n^{5/2}}{(n+1)!n\sqrt{\pi}}\left[\frac{3}{n^2-1}\right]^{1/2},\quad \lambda_n=Z/n \qquad (1''')$$

where $\phi_{np_{x,z}}(\vec{r}_2)$ represents the np_x or the np_z wave function for hydrogenlike ion and $r_{2x,z}$ denotes the x or the z component of the coordinate vector $\vec{r}_2$.

Here we have chosen the axis of quantization along the direction of $\vec{K}_i$ and the plane of scattering is taken to be the x-z plane. We now use the following integral representation[23] for the Laguerre polynomial in order to represent the final-state wave function:

$$L_m(\xi)=\frac{m!}{2\pi i}\oint_\Gamma\frac{\exp[-\xi t/(1-t)]}{(1-t)t^{m+1}}dt , \qquad (2)$$

where Γ is a closed contour enclosing the point $t=0$.

In view of the relation

$$L^{2l+1}_{n+l}(\xi)=\frac{\partial^{2l+1}L_{n+l}(\xi)}{\partial\xi^{2l+1}}$$

we get for the p state after the substitution $t=(x-1)/(x+1)$

$$L^3_{n+1}(2\lambda_nr_2)=-\frac{(n+1)!}{2\pi i}\oint_{\Gamma'}\exp[-\lambda_n(x-1)r_2]\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx , \qquad (3)$$

where Γ' is the closed contour enclosing the point $x=1$.

We now define

$$A_{x,z}(\vec{r}_1)=\int\phi_{np_{x,z}}(\vec{r}_2)\frac{1}{r_{12}}\phi_{1s}(\vec{r}_2)d\vec{r}_2 .$$

Using Eqs. (1″), (1‴), and (3) $A_{x,z}$ can be written as

$$A_{x,z}(\vec{r}_1)=N_{1s}N_{np}\frac{(n+1)!}{16\pi i}\oint_{\Gamma'}\left[\int r_{2x,z}\frac{e^{-\lambda r_2}}{r_{12}}d\vec{r}_2\right]\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx , \qquad (4)$$

where $\lambda=\lambda_1+\lambda_nx$.

After performing the space integration in Eq. (4) we arrive at

$$\vec{A}(\vec{r}_1)=-N_{1s}N_{np}\frac{(n+1)!}{4i}\oint_{\Gamma'}\left[\frac{1}{\lambda}\frac{\partial^2f}{\partial\lambda^2}-\frac{1}{\lambda^2}\frac{\partial f}{\partial\lambda}\right]\frac{\vec{r}_1}{r_1^3}\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx ,$$
$$f(r_1)=\int_0^{r_1}r'e^{-\lambda r'}dr' . \qquad (5)$$

We substitute the above expression for $\vec{A}(\vec{r}_1)$ in Eq. (1) and carry out the r_1 integration following closely the procedure adopted by Sung Dahm Oh *et al.*,[15] in their parallel case of $1s$-$2p$ transition and finally obtain

$$\vec{T}_{1s-np} = -\frac{N_{1s}N_{np}(n+1)!N_{K_i}N_{K_f}}{8\pi i(Z-1)} \oint_{\Gamma'} \left[\frac{1}{\lambda}\frac{\partial^2}{\partial\lambda^2} - \frac{1}{\lambda^2}\frac{\partial}{\partial\lambda}\right] \vec{I}\,\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx \;, \tag{6}$$

where

$$N_{K_i} = \exp\left[\pi\frac{Z-1}{2K_i}\right]\Gamma(1-a), \quad N_{K_f} = \exp\left[\pi\frac{Z-1}{2K_f}\right]\Gamma(1-b)$$

and

$$\vec{I} = \langle \vec{K}_f, b \mid [H, \vec{\nabla}] f(r_1) \mid \vec{K}_i, a \rangle \tag{6'}$$

with

$$| \vec{K}_i, a+n \rangle = e^{i\vec{K}_i\cdot\vec{r}_1}{}_1F_1(a+n, 1; i(K_i r_1 - \vec{K}_i\cdot\vec{r}_1)) \;,$$

$$| \vec{K}_f, b+n \rangle = e^{i\vec{K}_f\cdot\vec{r}_1}{}_1F_1(-(b+n), 1; -i(K_f r_1 + \vec{K}_f\cdot\vec{r}_1)) \;.$$

The expression $[H, \vec{\nabla}]$ occurring in Eq. (6′) denotes the commutator of the operators H and $\vec{\nabla}$. Expression (6) may equivalently be thrown into the form

$$\vec{T}_{1s-np} = -\frac{N_{1s}N_{np}(n+1)!N_{K_i}N_{K_f}}{8\pi i(Z-1)} \oint_{\Gamma'} \frac{\partial}{\partial\lambda}\left[\frac{1}{\lambda}\frac{\partial}{\partial\lambda}\right] \vec{I}\,\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx \;. \tag{7}$$

Taking the projections of $\vec{I}$ along the directions of $\hat{K}_i$ and $\hat{K}_f$ we obtain the x and z components of the transition amplitude $\vec{T}_{1s-np}$ as

$$T_x = C\oint_{\Gamma'} \frac{\partial}{\partial\lambda}\left[\frac{1}{\lambda}\frac{\partial}{\partial\lambda}\right] \vec{I}\cdot\hat{K}_i\,\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx \;, \tag{8a}$$

$$T_z = C\oint_{\Gamma'} \frac{\partial}{\partial\lambda}\left[\frac{1}{\lambda}\frac{\partial}{\partial\lambda}\right] \left[(\vec{I}\cdot\hat{K}_f - \cos\theta\,\vec{I}\cdot\hat{K}_i)\frac{1}{\sin\theta}\right] \frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx \;, \tag{8b}$$

where

$$C = -\frac{N_{1s}N_{np}(n+1)!N_{K_i}N_{K_f}}{8\pi i(Z-1)}$$

and $\cos\theta = \hat{K}_i\cdot\hat{K}_f$.

The expressions of $\vec{I}\cdot\hat{K}_i$ and $\vec{I}\cdot\hat{K}_f$ have been given by Sung Dahm Oh *et al.*[15] as

$$\vec{I}\cdot\hat{K}_i = \frac{a}{2}\left[\frac{K_i^2-K_f^2}{\lambda^2}[(I_{a+1,b}-I_{ab})_{\lambda=0} - (I_{a+1,b}-I_{ab})] + (I_{a+1,b}-I_{ab}) - \frac{2iK_i}{\lambda}I_{a+1,b}\right] , \tag{9a}$$

$$\vec{I}\cdot\hat{K}_f = \frac{b}{2}\left[\frac{K_i^2-K_f^2}{\lambda^2}[(I_{a,b+1}-I_{ab})_{\lambda=0} - (I_{a,b+1}-I_{ab})] - (I_{a,b+1}-I_{ab}) + \frac{2iK_f}{\lambda}I_{a,b+1}\right] , \tag{9b}$$

where

$$I_{ab} = \int \frac{e^{i\vec{q}\cdot\vec{r}_1}e^{-\lambda r_1}}{r_1}\,{}_1F_1(a,1;i(K_i r_1 - \vec{K}_i\cdot\vec{r}_1))\,{}_1F_1(b,1;i(K_f r_1 + \vec{K}_f\cdot\vec{r}_1))\,d\vec{r}_1 \;. \tag{10}$$

The integral I_{ab} has been evaluated analytically by Nordsieck[24] and may be written as

$$I_{ab} = \exp\left[-\pi\frac{Z-1}{2K_i}\right]\frac{2\pi}{\alpha}\left[\frac{\alpha}{\gamma}\right]^a\left[\frac{\gamma+\delta}{\gamma}\right]^{-b}{}_2F_1\left[1-a, b, 1; \frac{K_iK_f - \vec{K}_i\cdot\vec{K}_f}{\alpha}\right] \tag{11}$$

with

$$\alpha=\tfrac{1}{2}(q^2+\lambda^2),\quad \vec{q}=\vec{K}_i-\vec{K}_f,\quad \beta=\vec{K}_f\cdot\vec{q}-i\lambda K_f,\quad \gamma=\vec{K}_i\cdot\vec{q}-i\lambda K_i-\alpha,\quad \delta=K_iK_f+\vec{K}_i\cdot\vec{K}_f-\beta\ .$$

It should be noted that the form of the expression of I_{ab} in Eq. (11) differs from that of Sung Dahm Oh *et al.*[15] though they are completely equivalent.

We shall now present the calculation of T_z only, since the calculation of T_x is very similar to that of T_z.

Applying the method of integration by parts and noting that

$$\frac{1}{\lambda}\frac{\partial}{\partial\lambda}\vec{I}\cdot\hat{K}_i\left[\frac{x+1}{x-1}\right]^n$$

is a single-valued function over the closed contour, we obtain from Eq. (8a)

$$T_z=\frac{C}{\lambda_n}\oint_{\Gamma'}\frac{\partial}{\partial\lambda}\vec{I}\cdot\hat{K}_i\left[\frac{2}{\lambda}(x-n)\left[\frac{x+1}{x-1}\right]^n\right]dx\ .$$

Integrating by parts a second time we finally obtain

$$T_z=\frac{2C}{\lambda_n^2}\oint_{\Gamma'}\vec{I}\cdot\hat{K}_i\left\{\frac{1}{\lambda}\left[\frac{x+1}{x-1}\right]^n\left[(x-n)\left[\frac{\lambda_n}{\lambda}+\frac{2n}{x^2-1}\right]-1\right]\right\}dx\ . \tag{12}$$

Following Sinha *et al.*[14] the contour Γ' has been chosen to be a circle with a suitable radius ($x=ane^{i\phi}$). The integral (12) thus reduces to a one-dimensional integral over ϕ ranging from 0 to 2π:

$$T_z=\frac{i2Can}{\lambda_n^2}\int_0^{2\pi}\vec{I}\cdot\hat{K}_i\left\{\frac{1}{\lambda}\left[\frac{x+1}{x-1}\right]^n\left[(x-n)\left[\frac{\lambda_n}{\lambda}+\frac{2n}{x^2-1}\right]-1\right]\right\}e^{i\phi}d\phi\ . \tag{13}$$

B. Exchange amplitudes

In the CBO approximation one requires further evaluation of the exchange amplitude in addition to the direct one. The x and the z components of the exchange amplitudes are given by

$$g_{x,z}=\frac{1}{2\pi}\int\int\phi^*_{np_{x,z}}(\vec{r}_1)\psi^{(-)*}_{\vec{K}_f}(\vec{r}_2)\left[\frac{1}{r_{12}}-\frac{1}{r_1}\right]\phi_{1s}(\vec{r}_2)\psi^{(+)}_{\vec{K}_i}(\vec{r}_1)d\vec{r}_1d\vec{r}_2\ . \tag{14}$$

To evaluate $g_{x,z}$ we first start with the parent integral

$$V=\oint_{\Gamma'}\oint_{\Gamma_1}\oint_{\Gamma_2}\int\int e^{-\lambda_1 r_2}e^{-\eta r_1}e^{-i\vec{K}_f\cdot\vec{r}_2}e^{i\vec{\Delta}\cdot\vec{r}_1}\left[\frac{1}{r_{12}}-\frac{1}{r_1}\right]e^{i(K_fr_2+\vec{K}_f\cdot\vec{r}_2)t_2}e^{i(K_ir_1-\vec{K}_i\cdot\vec{r}_1)t_1}$$
$$\times\left[-\frac{1}{4\pi^2}p(\alpha_1,t_1)p(\alpha_2,t_2)\right]\frac{(x+1)^{n+1}}{(x-1)^{n-1}}d\vec{r}_1d\vec{r}_2dt_1dt_2dx\ , \tag{15}$$

where we have used the integral representation of ${}_1F_1$ as

$${}_1F_1(i\alpha_j,1;z)=\frac{1}{2\pi i}\int_{\Gamma_j}^{(0^+,1^+)}dt_jp(\alpha_j,t_j)e^{zt_j}$$

with

$$p(\alpha_j,t_j)=t_j^{i\alpha_j-1}(t_j-1)^{-i\alpha_j},\quad j=1,2\ .$$

Γ_j is a closed contour encircling the two points 0 and 1 once anticlockwise.

The integral $g_{x,z}$ may now be generated from V through the relation

$$g_{x,z}=\frac{C_1}{i}\left[\frac{\partial V}{\partial \Delta_{x,z}}\right]_{\vec{\Delta}=\vec{K}_i},\quad C_1=\frac{N_{1s}N_{np}(n+1)!N_{K_i}N_{K_j}}{32\pi^2 i}\;. \tag{16}$$

We call the two parts of V involving the potentials $1/r_{12}$ and $1/r_1$ as V_1 and V_2, respectively. Performing the space integrations in V_2 we obtain

$$V_2=-16\pi^2\frac{\partial}{\partial\lambda_1}\oint_{\Gamma'}\left[-\frac{1}{4\pi^2}\oint_{\Gamma_1}\oint_{\Gamma_2}\frac{dt_1 p(\alpha_1,t_1)dt_2 p(\alpha_2,t_2)}{(A_1-B_1t_1)(A_2-B_2t_2)}\right]\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx$$

$$=-16\pi^2\frac{\partial}{\partial\lambda_1}\oint_{\Gamma'}\left[\frac{1}{A_1}\left[1-\frac{B_1}{A_1}\right]^{-i\alpha_1}\frac{1}{A_2}\left[1-\frac{B_2}{A_2}\right]^{-i\alpha_2}\right]\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx\;, \tag{17a}$$

where

$$A_1=\Delta^2+\eta^2,\quad B_1=2(\vec{\Delta}\cdot\vec{K}_i+iK_i\eta),\quad A_2=K_f^2+\lambda_1^2,\quad B_2=2(K_f^2+iK_f\lambda_1)$$
$$\eta=\lambda_n x\;. \tag{17b}$$

The space integral in V_1 can be evaluated as the double derivative of the Lewis integral[25]

$$V_1=8\frac{\partial}{\partial\lambda_1}\frac{\partial}{\partial\eta}\oint_{\Gamma'}\left[-\frac{1}{4\pi^2}\oint_{\Gamma_1}\oint_{\Gamma_2}Lp(\alpha_1,t_1)p(\alpha_2,t_2)dt_1dt_2\right]\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx \tag{18}$$

with

$$L=\frac{\pi^2}{(\beta^2-\alpha\gamma)^{1/2}}\ln\left[\frac{\beta+(\beta^2-\alpha\gamma)^{1/2}}{\beta-(\beta^2-\alpha\gamma)^{1/2}}\right],$$

where

$$\beta=\lambda_1'(K_i'^2+\eta'^2)+\eta'(K_f'^2+\lambda_1'^2),\quad \alpha\gamma=[(\vec{K}_i'-\vec{K}_f')^2+(\eta'+\lambda_1')^2](K_i'^2+\eta'^2)(K_f'^2+\lambda_1'^2)\;,$$
$$\vec{K}_i'=\vec{K}_it_1-\vec{\Delta},\quad \vec{K}_f'=\vec{K}_ft_2-\vec{K}_f,\quad \lambda_1'=\lambda_1-iK_ft_2,\quad \eta'=\eta-iK_it_1\;.$$

We now use the integral representation of the Lewis integral L (Ref. 25)

$$L=2\pi^2\int_0^\infty dv\,(\alpha v^2+2\beta v+\gamma)^{-1}\;,$$

where we have split the product $\alpha\gamma$ in a manner such that α and γ are linear functions of t_1 and t_2. Thus we choose

$$\alpha=(\vec{K}_i'-\vec{K}_f')^2+(\eta'+\lambda_1')^2\;,$$
$$\gamma=(K_i'^2+\eta'^2)(K_f'^2+\lambda_1'^2)\;. \tag{19}$$

It may be noted that β is already a linear function in t_1 and t_2. Next we express α, β, and γ in the following form in order to perform the t_1 and t_2 integrations analytically:

$$\alpha=A+Bt_1+Ct_1t_2+Dt_2\;,$$
$$\beta=P+Qt_1+Rt_1t_2+St_2\;, \tag{20}$$
$$\gamma=E+Ft_1+Gt_1t_2+Ht_2\;,$$

where $A,B,C,\ldots$, etc., are functions of $\vec{K}_i$, $\vec{K}_f$, λ_1, and η only.

In view of Eqs. (19) and (20) L can be thrown into a form as used earlier by Sinha and Sil,[17]

$$L=-2\pi^2\int_0^\infty\frac{dv}{(V+W)t_1t_2+(U+Y)t_1-Vt_2-U}\;, \tag{21}$$

where U, V, W, and Y are functions of the constants $A,B,C,D,\ldots$, etc.

Substituting (21) for L in (18) we first carry out t_1 and t_2 integrations analytically, following the method of Nordsieck.[24] It is to be noted here that Nordsieck evaluated the integral of the type

$$J_0=-\frac{1}{4\pi^2}\oint_{\Gamma_1}\oint_{\Gamma_2}L(t_1,t_2)p(\alpha_1,t_1)p(\alpha_2,t_2)dt_1dt_2 \tag{22}$$

for some restricted values of the parameters. But our integral (18) is to be evaluated for any complex value of x within the contour Γ'. We have noted that our result may be obtained by an analytic continuation of the result of Nordsieck around the point $x=1$. We then arrive at the expression given below[17]:

$$J_0=2\pi^2\exp(-\pi\alpha_1)\int_0^\infty\left[U^{i\alpha_1-1}Y^{i\alpha_2-i\alpha_1}(Y+W)^{-i\alpha_2}\,{}_2F_1\left[1-i\alpha_1,i\alpha_2,1;\frac{UW-VY}{U(Y+W)}\right]\right]dv\ . \tag{23}$$

In view of Eqs. (23) and (18) the exchange integral involving the $1/r_{12}$ part now becomes

$$V_1=8\frac{\partial}{\partial\lambda_1}\frac{\partial}{\partial\eta}\oint_{\Gamma'}J_0\frac{(x+1)^{n+1}}{(x-1)^{n-1}}dx\ . \tag{24}$$

Using the relation (17b) and then applying the method of integration by parts we finally obtain from (24)

$$V_1=\frac{8}{\lambda_n}\frac{\partial}{\partial\lambda_1}\oint_{\Gamma'}2(n-x)\left[\frac{x+1}{x-1}\right]^n J_0dx\ . \tag{25}$$

This integral is then transformed to a one-dimensional ϕ integral as in the direct case. The differential cross section in the CBO approximation is given by

$$\frac{d\sigma_{x,z}}{d\Omega}=\frac{K_f}{K_i}\left(\tfrac{1}{4}\,|\,T_{x,z}+g_{x,z}\,|^2+\tfrac{3}{4}\,|\,T_{x,z}-g_{x,z}\,|^2\right)\ . \tag{26}$$

C. Asymptotic value of the scaled cross section

To evaluate the asymptotic scaled cross section we first note that in the limit $n\to\infty$ the excitation threshold energy becomes $\frac{1}{2}Z^2$ and the quantity $\lambda_n x$ on the contour $x=ane^{i\phi}$ is independent of n. Further, the final momentum $\vec{K}_f$ becomes a constant parameter and as a result $\vec{I}\cdot\hat{K}_i/\lambda$ becomes constant in the above limit. Thus we need consider the following limit only in Eq. (13):

$$\lim_{n\to\infty}\left[\frac{x+1}{x-1}\right]^n\left[(x-n)\left[\frac{\lambda_n}{\lambda}+\frac{2n}{x^2-1}\right]-1\right]=e^{2y}\left[(ae^{i\phi}-1)\left[\frac{Z}{\lambda}+\frac{2}{a^2e^{2i\phi}}\right]-1\right],$$

where

$$y=a^{-1}e^{-i\phi}\ .$$

Finally, in view of the n dependence of the normali-

TABLE I. Scaled cross sections (σn^3Z^4 in units of πa_0^2) for $1s$-np excitation of He^+ by electron impact. (a) CB cross section; (b) CBO singlet; (c) CBO triplet; (d) total CBO cross section.

Energy (Threshold units)		Excited levels 2p	3p	4p	∞p
1.5	(a)	13.32	7.568	6.327	5.088
	(b)	28.46	17.64	15.16	12.59
	(c)	5.643	2.689	2.138	1.621
	(d)	11.35	6.428	5.393	4.365
2.5	(a)	11.78	6.494	5.377	4.272
	(b)	18.27	10.47	8.771	7.072
	(c)	7.413	3.906	3.188	2.489
	(d)	10.13	5.546	4.584	3.634
3.5	(a)	10.32	5.582	4.595	3.626
	(b)	13.61	7.524	6.238	4.965
	(c)	7.839	4.142	3.383	2.645
	(d)	9.281	4.987	4.097	3.225

TABLE II. Scaled cross section ($\sigma n^3 Z^4$ in units of πa_0^2) for $1s$-np excitation of He^+ by electron impact in CB approximation.

Energy (Threshold units)	Excited levels 2p	3p	4p	5p	∞p
5	8.775	4.660	3.815	3.489	2.990
8	6.795	3.537	2.878	2.625	2.239
12	5.304	2.722	2.205	2.007	1.707

zation constant we obtain the amplitude proportional to $n^{-3/2}$. Limiting expressions for the exchange amplitudes in Eqs. (17a) and (25) can be obtained easily following the same procedure.

III. RESULTS AND DISCUSSIONS

The usual practice of repeated application of parametric differentiation to obtain the excitation cross section for higher n values has been avoided in the present work by one-dimensional integration. By virtue of our method it is possible to evaluate the $1s$-np excitation cross section of hydrogenlike ions for any arbitrary value of n, including the asymptotic limit ($n \rightarrow \infty$), at any energy through a general computer program with equal ease and precision. For a consistency check of our generalized program we have reproduced the CB results of Tully[4] for $2p$, $3p$, and $6p$ up to the figures quoted by him at several energies with $Z=2$ and 4. For the CBO results we have reproduced the $1s$-$2p$ cross section of Mitra and Sil[13] for $Z=2$ at double the threshold energy.

We have noticed that at an energy higher than four times the threshold, the CBO cross sections are nearly equal to the corresponding CB cross sections.

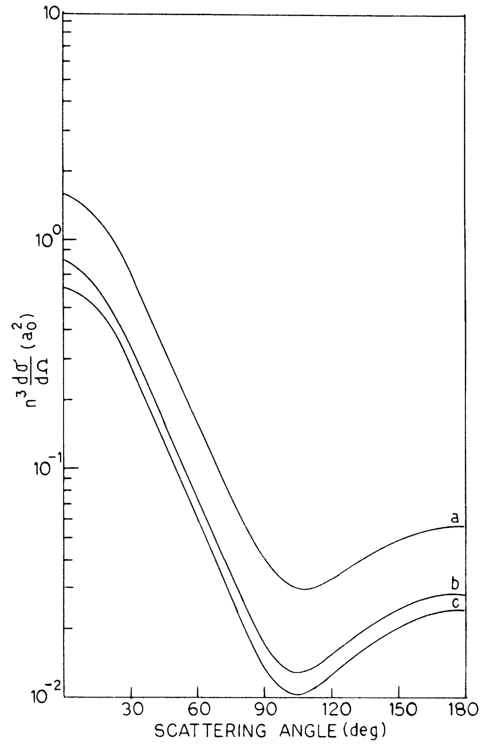

FIG. 1. Scaled differential cross sections $(d\sigma/d\Omega)n^3$ for the $1s$-np transition of He^+ by electron impact at an energy 1.5 times the threshold in the CBO approximation. a, $n=2$; b, $n=4$; c, $n=\infty$.

We have tabulated the CB and CBO results for a He^+ target at energies 1.5, 2.5, and 3.5 times the threshold energy for $n=2$, 3, 4, and ∞ in Table I. Beyond this energy region we have calculated only the CB cross sections up to 12 times the threshold for $n=2$, 3, 4, 5, and ∞ which are tabulated in Table II. In Table III we have presented the Fano-Macek alignment parameter (FMAP) $A_{col}=(0.5\sigma_x-\sigma_z)/(\sigma_x+\sigma_z)$ both in the CB and

TABLE III. Fano-Macek alignment parameter (FMAP) for $1s$-np excitation of He^+ by electron impact. I: FMAP in CB approximation; II: FMAP in CBO approximation.

Energy (Threshold units)		Excited levels 2p	3p	4p	∞p
1.5	I	−0.6216	−0.6241	−0.6246	−0.6250
	II	−0.6321	−0.6296	−0.6297	−0.6302
2.5	I	−0.4260	−0.4113	−0.4064	−0.4004
	II	−0.4169	−0.4026	−0.3980	−0.3923
3.5	I	−0.2912	−0.2720	−0.2658	−0.2582
	II	−0.2809	−0.2620	−0.2559	−0.2484

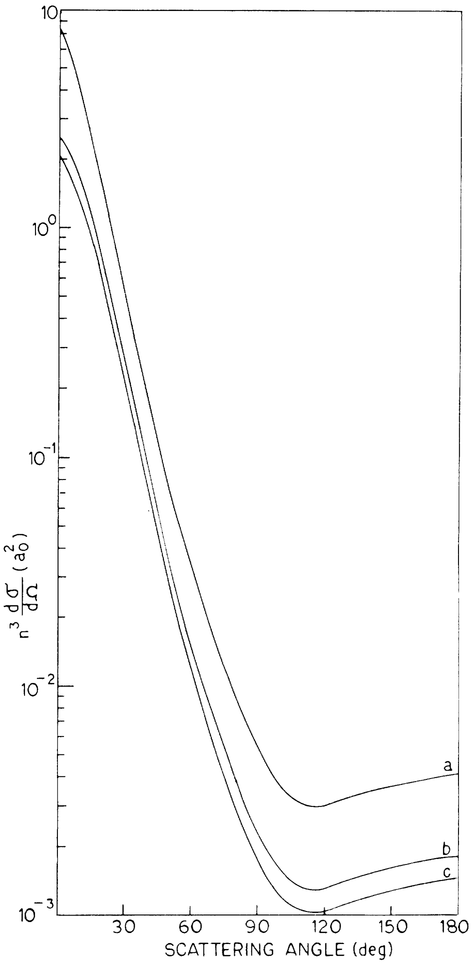

FIG. 2. Scaled differential cross sections $(d\sigma/d\Omega)n^3$ for the $1s$-np transition of He^+ by electron impact at an energy 2.5 times the threshold in the CBO approximation. a, $n=2$; b, $n=4$; c $n=\infty$.

CBO approximations. It is interesting to note that at 1.5 times the threshold energy, the FMAP in the CBO approximation is a little higher than the corresponding FMAP in the CB approximation for all values of n. But at energies 2.5 and 3.5 times the threshold, the situation is reversed. From our results of the total cross section and the corresponding FMAP one can find the x and z components of the total cross sections through the relations

$$\sigma_x = \frac{2}{3}\frac{\sigma_{sc}}{n^3Z^4}(1+A_{col}) ,$$

$$\sigma_z = \frac{1}{3}\frac{\sigma_{sc}}{n^3Z^4}(1-2A_{col}) , \quad \sigma_{sc}=\sigma n^3 Z^4 .$$

We have also studied the nature of the differential cross sections in CBO approximation for different values of n. We have plotted in Fig. 1 the n^3 differential cross sections for He^+ against the scattering angle at 1.5 times the threshold energy for $n=2$, 4, and ∞. Figure 2 exhibits the corresponding curves at 2.5 times the threshold energy. It may be noted that at 1.5 times the threshold energy the differential cross section rises in the backward direction after reaching a minimum near 110° while at an energy 2.5 times the threshold the minimum occurs near 115°. This rise in the backward direction may be attributed to the exchange effect. It was noted earlier[13] that the agreement of the CBO $1s$-$2p$ excitation cross section results with experiment[2] for e-He^+ was good enough even at an energy as low as 60 eV. This is in contrast with the $1s$-$2s$ CBO cross section results which grossly overestimate the experimental findings near the threshold energy. In electron-hydrogen excitation a similar feature was noted[26] for Born-Oppenheimer calculations, viz., the $1s$-$2p$ results were much better near the threshold region compared to the results of $1s$-$2s$ excitation. Thus we may expect that our $1s$-np results may provide a reasonably good estimate of the excitation cross sections for any value of n (including the limit $n\to\infty$) throughout the energy range considered here.

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