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Different forms of direct- and exchange-scattering amplitudes for the n_1s-n_2s transition in electron-hydrogen collisions

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A simple series-expansion form for the direct-scattering amplitude (involving real quantities) $T^d_{n_1s\text{-}n_2s}$ is given in the case of the n_1s-n_2s transition in the electron—hydrogen-atom collision. Another form for $T^d_{n_1s\text{-}n_2s}$, consisting of few terms, is derived when the initial-state quantum number n_1 is small. When the quantum numbers n_1 and n_2 are very large, the dominant part of $T^d_{n_1s\text{-}n_2s}$ can be reduced to a single oscillatory trigonometric term, and this leads to some interesting features of the differential cross section. Simple integral forms for $T^d_{n_1s\text{-}n_2s}$ in the above-mentioned cases are also given. Expressions are further obtained for the exchange-scattering amplitude $T^{\text{ex}}_{n_1s\text{-}n_2s}$, which includes terms of orders $O(\beta_0^{-1})$ and $O(\beta_0^{-2})$, with $\beta_0=k_1^2+n_2^{-2}=k_2^2+n_1^{-2}$, where k_1 (k_2) is the initial (final) electron momentum. We also derive exact expressions for $T^{\text{ex}}_{2s\text{-}2s}$ and $T^{\text{ex}}_{1s\text{-}3s}$. All calculations are done in the first Born approximation.

I. INTRODUCTION

A general expression of the direct-scattering amplitude for the n_1s-n_2s transition is presented in the form of a series "expansion" expressed as a function of momentum transfer Δ in the case of the electron—hydrogen-atom collision. This series converges rapidly as Δ increases. The different coefficients of the above expansion are determined by evaluating certain series characterized by n_1 and n_2. For large values of n_1 and n_2 these coefficients are reduced to very simple expressions. The present calculation for the scattering amplitude also holds for transitions involving high Rydberg states (having large quantum numbers n) of atoms other than hydrogen since these states can be assumed to be hydrogenic. The scattering amplitude can be alternately expressed as a double integral over the range 0—2π for finite values of n_1 and n_2 and as a simple form of single integral only when both n_1 and n_2 become infinitely large and Δ is not too small. For $n_1\to\infty$, $n_2\to\infty$, and Δ values that are not small the scattering amplitude can also be expressed in terms of a dominant part, which is proportional to $\sin^2(4/\Delta)$, and the remaining part, consisting of small terms. This shows that for not very small Δ, different maxima in the expression for the scattering cross section are almost equally spaced when plotted as a function of $1/\Delta$ and furthermore, the cross section monotonously decreases for Δ about greater than $8/\pi$. All the maxima of differential cross sections in these cases can further be grouped into two distinct series of maxima, which will be discussed in detail in Sec. IV. We also give some compact expressions for the direct-scattering amplitude for $1s$-ns and $2s$-ns transitions involving few terms both for finite and infinite values of n. We mention that Saha and Sil[1] have expressed the n_1s-n_2s scattering amplitude in the form of a hypergeometric function where the variable is a complicated quantity involving four factors which are complex quantities and depend upon Δ, n_1^{-1}, and n_2^{-1}. In contrast, our results are explicitly expressed in terms of real quantities having a simple dependence on Δ. Saha and Sil[1] have not done any detailed numerical calculations based on their results, as was done in this paper. We also note that Massey and Mohr[2] have given a different form of the scattering amplitude in the particular case of a transition from a ground state to an excited state. In this case, Landau and Lifshitz[3] have used parabolic coordinates to express their result in terms of appropriate parabolic quantum numbers.

It may be noted that the evaluation of the exchange-scattering amplitude for the simplest system of an electron scattered by a hydrogen atom in the first Born approximation is much more difficult than that for the direct-scattering amplitude, as it involves six-dimensional integrations which have been evaluated in closed form by Corinaldesi and Trainor[4] in the case of $1s$-$1s$, $1s$-$2s$, and $1s$-$2p$ transitions. Using their procedure we calculate exchange-scattering amplitudes for the particular cases of $2s$-$2s$ and $1s$-$3s$ transitions. The above-mentioned exchange integrals have been simplified by Ochkur[5] by expanding the exchange-scattering amplitude (given in first-order formulation) in inverse powers of the momentum of the projectile electron and retaining terms of lowest order. The general formula for first-order exchange-scattering amplitude for the n_1s-n_2s transition as derived in this paper is expressed in a form so as to include terms (depending upon momentum transfer) of $O(\beta_0^{-1})$ and $O(\beta_0^{-2})$ where $\beta_0=k_1^2+n_2^{-2}=k_2^2+n_1^{-2}$. We may point out that the derivation of explicit expressions for both direct- and exchange-scattering amplitudes in the case of n_1s-n_2s transition is carried out by taking appropriate combinations of repeated parametric differentiations[6] of a "characteristic function." The above-mentioned term of $O(\beta_0^{-1})$ corresponds to the usual Ochkur[5] approximation. Shakeshaft[7] has given an approximate form for the correction term (in first-order calculation) to the Ochkur[5] approximation, which corresponds to a term of $O(\beta_0^{-2})$ as evaluated in this paper. He has further approximately evaluated second Born correction terms in the case of 1s-1s and 1s-2s transitions and has shown that these correction terms have greater contributions than the usual Ochkur[5] term, especially in the forward direction. In our numerical calculation we have found that the term of $O(\beta_0^{-2})$ (as determined in the present paper) receives increasingly significant contributions compared to the usual Ochkur[5] approximation [of $O(\beta_0^{-1})$] term as the momentum transfer increases. Some investigators[8–10] have improved upon Ochkur's[5] method by adopting Glauber's[11] eikonal approximation procedure so as to account for the usual distortion of plane waves as used in Ochkur's[5] approximate treatment. Byron and Joachain[8] have investigated the range of validity of first-order calculations (as done in this paper) as compared with the numerical calculation based on the eikonal approximation (which contains contributions from all orders of perturbation theory) for the inelastic exchange-scattering process $e^- + \mathrm{He}(1\,^1S) \rightarrow e^- + \mathrm{He}(2\,^3S)$. They have observed that the eikonal correction to the first-order Born approximation result (as discussed in this paper) decreases with an increase in either projectile energy or scattering angle. At 500 eV incident electron energy they have found that at 10° and 15° the eikonal results agree well with the Born approximation, although at smaller angles, 0° and 5°, the differences are quite appreciable.

Recent advances[12,13] in experimental techniques for the production of polarized electron projectiles, polarized atomic targets, and the detection of polarization of the colliding system and sometimes also of the emitted photon after the collision enable us to investigate experimentally both (spin) exchange scattering and direct scattering in electron-atom collisions. Laser-excited atomic beams also provide us with a method[14,15] to study scattering processes (superelastic) for which $n_1 > n_2$ in n_1s-n_2s transition.

II. DIRECT-SCATTERING AMPLITUDE

The direct-scattering amplitude for the s-state transition $n_1s \rightarrow n_2s$ in electron—hydrogen-atom collision is given by

$$T^d_{n_1s\text{-}n_2s} = (2\pi)^{-3} \int e^{i\vec{\Delta}\cdot\vec{r}_0} \Psi^*_{n_2}(r_1) \left[\frac{1}{r_{01}} - \frac{1}{r_0} \right] \times \Psi_{n_1}(r_1)\, d\vec{r}_0 d\vec{r}_1 \,. \tag{2.1}$$

In (2.1) $\Psi_{n_1}(r_1)$ and $\Psi_{n_2}(r_1)$ are initial and final bound-state wave functions and $1/r_{01} - 1/r_0$ is the interaction potential, and the momentum transfer is

$$\vec{\Delta} = \vec{k}_1 - \vec{k}_2 \,. \tag{2.2}$$

The hydrogenic s-state wave function Ψ_{n_1s} is given by

$$\Psi_{n_1} = N_{n_1} e^{-r\lambda_1} \mathscr{L}^1_{n_1}(2r\lambda_1) \,, \tag{2.3}$$

where the normalization constant for the n_1s-state wave function, N_{n_1}, is

$$N_{n_1} = \frac{1}{\sqrt{4\pi}} \frac{2}{n_1^{3/2} n_1 n_1!} \,.$$

Now a typical term of the associated Laguerre polynomial $\mathscr{L}^1_{n_1}(2r\lambda_1)$ in Eq. (2.3), $r^p e^{-\lambda_1 r}$ can be written[6] as $(-1)^p (d/d\lambda_1)^p e^{-r\lambda_1}$. This enables us to express Ψ_{n_1s} in the following form involving parametric differentiations:[6]

$$\Psi_{n_1} = N_{n_1} n_1 n_1! \sum_{p_1=0}^{n_1-1} F^{(n_1)}_{p_1} \left[\frac{d}{d\lambda_1} \right]^{p_1} e^{-r\lambda_1} \,. \tag{2.4}$$

In (2.4) we have

$$F^{(n_1)}_{p_1} = \left[\frac{2}{n_1} \right]^{p_1} \frac{(n_1-1)!}{(n_1-1-p_1)!\, p_1!\, (p_1+1)!} \tag{2.5}$$

and

$$\lambda_1 = 1/n_1 \,. \tag{2.6}$$

A. Direct-scattering amplitude $T^d_{n_1s\text{-}n_2s}$ for the n_1s-n_2s transition

Using the relation

$$\begin{aligned}
(2\pi)^{-3} & \int e^{i\vec{\Delta}\cdot\vec{r}_0} \frac{1}{r_{01}} e^{-r_1\lambda} d\vec{r}_0 d\vec{r}_1 \\
&= (2\pi)^{-3} \int \frac{e^{i\vec{\Delta}\cdot(\vec{r}_0-\vec{r}_1)}}{r_{01}} e^{i\vec{\Delta}\cdot\vec{r}_1 - \lambda r_1} d\vec{r}_0 d\vec{r}_1 \\
&= (2\pi)^{-3} \frac{4\pi}{\Delta^2} \int e^{i\vec{\Delta}\cdot\vec{r}_1 - \lambda r_1} d\vec{r}_1 \\
&= -\frac{2}{\pi\Delta^2} \frac{\partial}{\partial\lambda} \left[\frac{1}{\lambda^2+\Delta^2} \right]
\end{aligned} \tag{2.7}$$

and those given by (2.1) and (2.4) we obtain for $n_1 \neq n_2$

$$T^d_{n_1s\text{-}n_2s} = -\frac{1}{2\pi\Delta^2} N_{n_1} N_{n_2} n_1 n_2 n_1! n_2! \times \sum_{p_1=0}^{n_1-1} \sum_{p_2=0}^{n_2-1} F^{(n_1)}_{p_1} F^{(n_2)}_{p_2} \left[\frac{d}{d\lambda} \right]^{p_1+p_2+1} \times \left[\frac{1}{\lambda^2+\Delta^2} \right] \tag{2.8}$$

which involves repeated parametric differentiation of the characteristic function given by (2.7), where λ in (2.8) is given by

$$\lambda = \lambda_1 + \lambda_2 = \frac{1}{n_1} + \frac{1}{n_2} \,. \tag{2.9}$$

Let us define the function

$$\begin{aligned}
g_p &= \left[\frac{d}{d\lambda} \right]^p \left[\frac{1}{\lambda^2+\Delta^2} \right] \\
&= -\frac{1}{2i\Delta} \left[\frac{d}{d\lambda} \right]^p (-\tilde{\Lambda} + \tilde{\Lambda}^*) \,,
\end{aligned} \tag{2.10}$$

where

$$\tilde{\Lambda}=-1/(\lambda+i\Delta)\ . \tag{2.11}$$

Then

$$\begin{aligned} g_p&=\frac{1}{2i\Delta}p![\tilde{\Lambda}^{p+1}-(\tilde{\Lambda}^*)^{p+1}]\\ &=(-1)^p\frac{p!}{\Delta}\left[\frac{1}{\lambda^2+\Delta^2}\right]^{(p+1)/2}\\ &\quad\times\sin\left[(1+p)\tan^{-1}\frac{\Delta}{\lambda}\right]. \end{aligned} \tag{2.12}$$

The direct-scattering amplitude can now be written as the following series summation:

$$T^d_{n_1s\text{-}n_2s}=-\frac{1}{2\pi^2\Delta^2}\left[\frac{4}{(n_1n_2)^{3/2}}\sum_{r=0}^{n_1+n_2-2} g_{r+1}F_r^{(n_1,n_2)}+\delta_{n_1n_2}\right]. \tag{2.13}$$

We note that the $1/r_0$ term of the interaction potential does not contribute to the integral of Eq. (2.1) or to the expression given by (2.8) because of the orthogonality of $\Psi_{n_1}(r_1)$ and $\Psi_{n_2}(r_1)$ when $n_1\neq n_2$. However, the term involving $\delta_{n_1n_2}$ in (2.13) corresponds to the $1/r_0$ part of the interaction potential which contributes to scattering amplitude when the initial and final-bound-state wave functions are identical. In (2.13) g_{r+1} is defined by the relation (2.12) and the associated numerical coefficient (independent of Δ) is given by

$$F_r=\sum_{p_1}\sum_{p_2=r-p_1}F_{p_1}^{(n_1)}F_{p_2}^{(n_2)}\ . \tag{2.14}$$

For small values of n_1 and n_2, the relation (2.13) for $T^d_{n_1s\text{-}n_2s}$ is simple enough. We can also represent $T^d_{n_1s\text{-}n_2s}$ by the following form involving the double integral $(n_1\neq n_2)$:

$$T^d_{n_1s\text{-}n_2s}=-\frac{2}{\pi^2\Delta^2}\frac{1}{(n_1n_2)^{3/2}}\frac{1}{2i\Delta}(L-L^*)\ , \tag{2.15}$$

where

$$L=\sum_{r=0}^{n_1+n_2-2}\tilde{\Lambda}^{r+2}(r+1)!F_r \tag{2.16}$$

$$=\left[\frac{1}{2\pi}\right]^2\int_0^{2\pi}\int_0^{2\pi}\left[1+\frac{2}{n_1}\tilde{\Lambda}e^{-iy}k\right]^{n_1-1}\left[1+\frac{2}{n_2}\tilde{\Lambda}e^{-iz}k\right]^{n_2}\left[1-\frac{e^{iy}+e^{iz}}{k}\right]^{-1}\frac{\tilde{\Lambda}}{2}e^{-iy}e^{iz}dy\,dz\ . \tag{2.17}$$

In (2.17) we assume $k>2$. Keeping in mind the relations (2.14) and (2.5) we have also

$$\begin{aligned} F_r&=\sum_{p_1,p_1',p_2}\frac{1}{2(r+1)!}\frac{(n_1-1)!}{(n_1-p_1-1)!p_1!}\left[\frac{2}{n_1}\right]^{p_1}\frac{n_2!}{(n_2-p_2-1)!(p_2+1)!}\left[\frac{2}{n_2}\right]^{p_2+1}\frac{(r+1)!}{(p_1'+1)!(r+1-p_1'-1)!}\\ &\quad\times\left[\frac{1}{2\pi}\right]\int_0^{2\pi}e^{-i(p_2+1-r-1+p_1'+1-1)z}dz\left[\frac{1}{2\pi}\right]\int_0^{2\pi}e^{-i(p_1-p_1'-1+1)y}dy\\ &=\frac{1}{2(r+1)!}\int_0^{2\pi}\int_0^{2\pi}\left[1+\frac{2}{n_1}e^{-iy}\right]^{n_1-1}\left[1+\frac{2}{n_2}e^{-iz}\right]^{n_2}(e^{iy}+e^{iz})^{r+1}e^{-iy}e^{iz}dy\,dz/(2\pi)^2\ . \end{aligned} \tag{2.18}$$

B. $T^d_{n_1s\text{-}n_2s}$ for $n_1,n_2\to\infty$

When both n_1 and n_2 are infinitely large and r $(=p_1+p_2)$ is small compared to n_1 or n_2, F_r defined by (2.14) and (2.5) can be replaced by

$$\begin{aligned} F_r^\infty&=\sum_{p_1}\sum_{p_2=r-p_1}\frac{2^r}{p_1!(p_1+1)!p_2!(p_2+1)!}\\ &=\frac{1}{2\pi}\frac{2^r}{[(r_1+1)!]^2}\int_0^{2\pi}(1+e^{i\phi})^{r+1}\\ &\qquad\times(1+e^{-i\phi})^{r+1}e^{i\phi}d\phi \end{aligned} \tag{2.19}$$

$$=\frac{2^{3r+2}}{r!(r+2)!}\frac{(2r+1)!!}{(2r+2)!!} \tag{2.20}$$

keeping in mind the fact that $(n_i-1)!/[n_i^{p_i}(n_i-1-p_i)!]\approx 1$ for $p_i\ll n_i$ $(i=1,2)$. In the above case L occurring in (2.15) is replaced by L^∞ $(=L$ for $n_1,n_2\to\infty$ or equivalently $\lambda\to 0)$. Using (2.16), (2.11) for $\lambda\to 0$, and (2.19) we can write

$$L^\infty=\frac{i}{2\Delta}\int_0^{2\pi}\exp\left[\frac{8i}{\Delta}\cos^2\frac{\phi}{2}\right]e^{i\phi}d\phi/2\pi \tag{2.21}$$

if the contribution from terms for values of $r\ll n_1+n_2-2$ (where $n_1\to\infty$, $n_2\to\infty$, or $\lambda\to 0$) to the exact value of $T^d_{n_1s\text{-}n_2s}$ is much greater than that from the remaining terms in (2.13), and this is possible if Δ occurring in the expression for (2.12) and (2.13) is not very small. In the above case the direct-scattering amplitude is given by the following single integral for $n_1,n_2\to\infty$:

$$T^d_{n_1s\text{-}n_2s}=-\frac{1}{\pi^2\Delta^4}\frac{1}{(n_1n_2)^{3/2}}\times\int_0^{2\pi}\cos\left[\frac{8\cos^2(\phi/2)}{\Delta}\right]\cos\phi\,d\phi/2\pi\ . \tag{2.22}$$

We obtain another reduced form of $T^d_{n_1s\text{-}n_2s}$ for infinitely large values of n_1 and n_2 or equivalently $\lambda\to0$ by keeping in mind the following facts. In the expression for F_r^∞ given by (2.20) the variation of the factor $(2r+1)!!/(2r+2)!!$ with r becomes very small beyond some very large value of r, say s $(=2s'+1)$. The quantity $1/[r!(r+2)!]$ in (2.20) tends to the value $1/[(r+1)!]^2$ when r becomes large. Using the above facts, the relation $\tan^{-1}(\Delta/\lambda)\to\pi/2$ as $\lambda\to0$, and the equations (2.12), (2.13), and (2.20), we obtain approximately when Δ is not very small and for $\lambda\to0$

$$T^d_{n_1s\text{-}n_2s}\simeq\frac{2}{\pi^2\Delta^4}\frac{1}{(n_1n_2)^{3/2}}\frac{(4s'+3)!!}{(4s'+4)!!}\left[\sin^2\left[\frac{4}{\Delta}\right]+\sum_{r'\geq0}^{s'}(-1)^{r'}\left[\frac{8}{\Delta}\right]^{2r'+2}\frac{1}{2}\frac{1}{(2r'+1)!}\frac{1}{(2r'+2)}\times\left[\frac{(2r'+2)}{(2r'+3)}\frac{(4r'+3)!!}{(4r'+4)!!}\frac{(4s'+4)!!}{(4s'+3)!!}-1\right]\right]\ . \tag{2.23}$$

The relation (2.23) has interesting consequences to be discussed in Sec. IV.

C. $T^d_{1s\text{-}ns}$ and $T^d_{2s\text{-}ns}$

For small values of n_1, $T^d_{n_1s\text{-}n_2s}$ is expressed in the following alternative form with the help of the relations (2.5) and (2.8):

$$T^d_{n_1\text{-}n_2s}=N_{n_1}N_{n_2}n_2n_2!n_1n_1!\left[\frac{n_2}{2}\right]^2\frac{1}{2i\Delta}\times\sum_{p_1=0}^{n_1-1}F^{(n_1)}_{p_1}\left[\frac{d}{d\lambda}\right]^{p_1}[\Lambda^2(1+\Lambda)^{n_2-1}-\text{c.c.}]\ , \tag{2.24}$$

where

$$\Lambda=\frac{2}{n_2}\tilde\Lambda \tag{2.25}$$

and c.c. stands for complex conjugate. From (2.24) we obtain

$$T^d_{1s\text{-}n_2s}=N_1N_{n_2}n_2n_2!\left[\frac{n_2}{2}\right]^2\frac{1}{\Delta}X_{\lambda,0} \tag{2.26}$$

and

$$T^d_{2s\text{-}n_2s}=4N_2N_{n_2}n_2n_2!\left[\frac{n_2}{2}\right]^2\frac{1}{\Delta}\left[X_{\lambda,0}+\frac{1}{2}\frac{n_2}{2}X_{\lambda,1}\right]\ , \tag{2.27}$$

where

$$X_{\lambda,0}=|\Lambda|^2\,|1+\Lambda|^{n_2-1}\sin[-2A+(n_2-1)B] \tag{2.28}$$

and

$$X_{\lambda,1}=-2|\Lambda|^3\,|1+\Lambda|^{n_2-1}\sin[-3A+(n_2-1)B]+(n_2-1)|\Lambda|^4\,|1+\Lambda|^{n_2-1}\times\sin[-4A+(n_2-2)B]\ . \tag{2.29}$$

A and B occurring in above equations are

$$A=\tan^{-1}(\Delta/\lambda)\ , \tag{2.30}$$

$$B=\tan^{-1}[\Lambda_I/(1+\Lambda_R)]\ , \tag{2.31}$$

where

$$\Lambda_R=\left[\frac{2}{n_2}\right]\tilde\Lambda_R=-\left[\frac{2}{n_2}\right]\frac{\lambda}{(\lambda^2+\Delta^2)} \tag{2.32}$$

and

$$\Lambda_I=\left[\frac{2}{n_2}\right]\tilde\Lambda_I=\left[\frac{2}{n_2}\right]\frac{\Delta}{(\lambda^2+\Delta^2)}\ ; \tag{2.33}$$

when $n_2\to\infty$ we have

$$T_{1s\text{-}n_2s}=N_1N_{n_2}n_2n_2!\exp(2\tilde\Lambda_R)Y_{\lambda,0} \tag{2.34}$$

and

$$T_{2s\text{-}n_2s}=4N_2N_{n_2}n_2n_2!\exp(2\tilde\Lambda_R)(Y_{\lambda,0}+\tfrac{1}{2}Y_{\lambda,1})\ , \tag{2.35}$$

where

$$Y_{\lambda,0}=|\tilde\Lambda|^2\sin(-2A-2\tilde\Lambda_I) \tag{2.36}$$

and

$$Y_{\lambda,1}=2[-|\tilde\Lambda|^3\sin(-3A+2\tilde\Lambda_I)+|\tilde\Lambda|^4\sin(-4A+2\tilde\Lambda_I)]\ . \tag{2.37}$$

III. EXCHANGE-SCATTERING AMPLITUDE

In the case of exchange scattering for the n_1s-n_2s transition, Joachain[16] has observed that if one neglects multiple scattering terms one can tentatively write, to first order in the interaction $1/r_{12}$, the following expressions for exchange-scattering amplitude:

$$T^{ex}_{n_1s\text{-}n_2s}\simeq(2\pi)^{-3}\langle\exp(i\vec k_2\cdot\vec r_2)\Psi_{n_2}(r_1)\,|\,r_{12}^{-1}\times|\exp(i\vec k_1\cdot\vec r_1)\Psi_{n_1}(r_2)\rangle\ . \tag{3.1}$$

Taking the Fourier transform of $1/r_{12}$ in momentum space one gets for the 1*s*-1*s* transition

$$T^{\rm ex}_{1s\text{-}1s}=T^{\rm ex}_{1s\text{-}1s}(\lambda_1,\lambda_2)\,|_{\lambda_1=\lambda_2=1}=\left[\frac{4}{\pi^4}\right]\tilde{A}\,|_{\lambda_1=\lambda_2=1}\ , \tag{3.2}$$

where

$$\tilde{A}=\frac{1}{4\lambda_1\lambda_2}\frac{\partial}{\partial\lambda_1}\frac{\partial}{\partial\lambda_2}\bar{A}\ . \tag{3.3}$$

Following the procedure of Lewis[17] we can write the function $\bar{A}$ occurring in (3.3) in the following form:

$$\bar{A}=\int\frac{d\vec{p}}{p^2[\lambda_1^2+(\vec{p}-\vec{k}_2)^2][\lambda_3^2+(\vec{p}-\vec{k}_1)^2]}=-2\pi^2CD\ , \tag{3.4}$$

where

$$C=1/X\ , \tag{3.5}$$

$$D=-\tan^{-1}(X/\beta)=-\frac{\pi}{2}+\tan^{-1}(\beta/X)\ , \tag{3.6}$$

$$\beta=\lambda_1(k_1^2+\lambda_2^2)+\lambda_2(k_2^2+\lambda_1^2)\ , \tag{3.7}$$

and

$$X^2=\Delta^2(k_1^2+\lambda_2^2)(k_2^2+\lambda_1^2)+(\lambda_1^2k_1^2-\lambda_2^2k_2^2)(k_2^2+\lambda_1^2-k_1^2-\lambda_2^2)\ . \tag{3.8}$$

The above relations lead to the following useful compact form for $X^2+\beta^2$:

$$X^2+\beta^2=(k_1^2+\lambda_2^2)(k_2^2+\lambda_1^2)[\Delta^2+(\lambda_1+\lambda_2)^2]\ . \tag{3.9}$$

A. Exchange-scattering amplitudes $T^{\rm ex}_{n_1s\text{-}n_2s}$ for n_1s-n_2s transition

Using (2.4) for the hydrogenic wave function we can calculate exchange-scattering amplitude $T^{\rm ex}_{n_1s\text{-}n_2s}$ by taking appropriate parametric differentiations of the characteristic function given by (3.4) [as in the derivation of the relation (2.13) for $T^{d}_{n_1s\text{-}n_2s}$] and consequently of the quantities C, D, β, X^2, and $1/(X^2+\beta^2)$. We obtain

$$\begin{aligned}T^{\rm ex}_{n_1s\text{-}n_2s}&\left[-\frac{2}{\pi^2}\frac{1}{(n_1n_2)^{3/2}}\right]^{-1}\\
&=\sum_r\left\{\frac{1}{\beta_0}(g_rF_{r-1})+\frac{g_r}{\beta_0^2}\left[(\Delta^2+\lambda^2)F_{r-1}+\lambda\left[\frac{4\lambda_1\lambda_2}{\Delta^2}+\tfrac{3}{2}r+2\right]F_r+\left[\frac{4\lambda_1\lambda_2(r+2)+2\lambda^2(r+1)}{\Delta^2}+(r+1)(r+2)\right]F_{r+1}\right.\right.\\
&\qquad+\frac{2\lambda(r+2)^2}{\Delta^2}F_{r+2}+\frac{2\lambda(\lambda_2-\lambda_1)}{\Delta^2}\tilde{F}_{r+1}-2\frac{(\lambda_1-\lambda_2)(r+2)}{\Delta^2}\tilde{F}_{r+2}\\
&\qquad\left.\left.-G_{r+1}+\frac{4\lambda}{\Delta^2}G_{r+2}+\frac{4(r+2)}{\Delta^2}G_{r+3}\right]+\frac{h_r}{\beta_0^2}[-(\lambda_1-\lambda_2)^2(r+1)F_{r+1}-(\lambda_1-\lambda_2)(r+1)\tilde{F}_{r+2}]\right\}\\
&\quad+\frac{4}{\beta_0^2\Delta^3}D_{n_1n_2}[\lambda_1\lambda_2F_0+\tfrac{1}{2}\lambda F_1-\tfrac{1}{2}(\lambda_1-\lambda_2)\tilde{F}_1+G_2]\ ,\end{aligned} \tag{3.10}$$

where

$$D_{n_1n_2}=-\frac{\pi}{2}+\tan^{-1}\frac{\lambda_1+\lambda_2}{\Delta}=-\tan^{-1}\frac{\Delta}{\lambda}\ , \tag{3.11}$$

$$\tilde{F}_r=\sum_{p_1}\sum_{p_2=r-p_1}(p_1-p_2)F^{(n_1)}_{p_1}F^{(n_2)}_{p_2}\ , \tag{3.12}$$

$$G_r=\sum_{p_1}\sum_{p_2=r-p_1}p_1p_2F^{(n_1)}_{p_1}F^{(n_2)}_{p_2}\ , \tag{3.13}$$

$$h_r=-\frac{1}{2\Delta}\frac{\partial}{\partial\Delta}g_r=\frac{(-1)^r r!}{2\Delta^2(\Delta^2+\lambda^2)^{(r+1)/2}}\left[\frac{1}{\Delta}\sin\left[(r+1)\tan^{-1}\frac{\Delta}{\lambda}\right]-\frac{(r+1)}{(\Delta^2+\lambda^2)^{1/2}}\cos\left[(r+2)\tan^{-1}\frac{\Delta}{\lambda}\right]\right]\ , \tag{3.14}$$

and

$$\beta_0=k_1^2+\lambda_2^2=k_2^2+\lambda_1^2\ . \tag{3.15}$$

The quantities F_r and g_r occurring in (3.10) are defined by (2.14) and (2.12).

For infinitely large values of n_1,n_2 and for a not very small value of Δ, the expression for exchange-scattering amplitude reduces to the form

$$T^{\rm ex}_{n_1s\text{-}n_2s} \simeq -\frac{2}{\pi^2}\frac{1}{(n_1n_2)^{3/2}}\left[\frac{1}{\beta_0}g_rF^{\infty}_{r-1}+\frac{g_r}{\beta_0^2}\left[\Delta^2F^{\infty}_{r-1}+(r+1)(r+2)F^{\infty}_{r+1}-G^{\infty}_{r+1}+\frac{4(r+2)}{\Delta^2}G^{\infty}_{r+3}\right]-\frac{\pi}{2}\frac{4}{\beta_0^2\Delta^3}G_2^{\infty}\right], \tag{3.16}$$

where

$$G_r^{\infty}=f^{(r)}_{\tau=0}-(r+1)f^{(r)}_{\tau=1}\ . \tag{3.17}$$

In (3.17) $f_\tau^{(r)}$ is given by

$$f_\tau^{(r)}=\frac{2^r}{r!(r+2\tau)!}\frac{1}{2\pi}\int_0^{2\pi}(1+e^{i\phi})^r(1+e^{-i\phi})^{r+2\tau}e^{i\tau\phi}d\phi \tag{3.18}$$

$$=2^{3r+2\tau}\frac{(2r+2\tau-1)!!}{(2r+2\tau)!!r!(r+2\tau)!!}\ . \tag{3.19}$$

The quantity F_r^{∞} occurring in (3.16) was already given by (2.20). We have also

$$F_r^{\infty}=f^{r}_{\tau=1}\ . \tag{3.20}$$

B. $T^{\rm ex}_{2s\text{-}2s}$ and $T^{\rm ex}_{1s\text{-}3s}$

Using the relation (2.4) to generate the $2s$-state wave function and the relations (3.3) and (3.4) we obtain the exact expression for the exchange elastic scattering amplitude in first-order approximation for the metastable $2s$ state of hydrogen:

$$\begin{aligned}T^{\rm ex}_{2s\text{-}2s}&=\frac{1}{2\pi^4}\left[1+\frac{1}{2}\frac{\partial}{\partial\lambda_1}\right]\left[1+\frac{1}{2}\frac{\partial}{\partial\lambda_2}\right]\bar{A}\Big|_{\lambda_1=\lambda_2=1/2}\\
&=\left[-\frac{1}{4\pi^2}\right]\left\{\left[\frac{8}{\beta}\left[-\frac{2}{\alpha^2}+\frac{7}{\alpha^3}-\frac{6}{\alpha^4}\right]+\frac{8}{\beta^2}\left[\frac{2}{\Delta^2}-\frac{2}{\alpha}+\frac{3}{\alpha^2}-\frac{2}{\alpha^3}\right]\right.\right.\\
&\quad+\frac{1}{\beta^3}\left[-\frac{19}{\Delta^2}+\frac{9}{\Delta^4}+\frac{15}{\alpha}-\frac{6}{\alpha^2}\right]+\frac{3}{\beta^4}\left[\frac{2}{\Delta^2}-\frac{3}{2\Delta^4}-\frac{1}{\alpha}\right]+\frac{9}{16}\frac{1}{\beta^5}\left[-\frac{1}{\Delta^2}+\frac{1}{\Delta^4}\right]\Bigg]\\
&\quad+\frac{D_{22}}{\Delta}\left[\frac{16}{\beta^2}\frac{1}{\Delta^2}+\frac{1}{\beta^3}\left[8-\frac{16}{\Delta^2}+\frac{9}{\Delta^4}\right]+\frac{3}{\beta^4}\left[-1+\frac{2}{\Delta^2}-\frac{3}{2\Delta^4}\right]\right.\\
&\quad\left.\left.+\frac{3}{8}\frac{1}{\beta^5}\left[\frac{3}{2}-\frac{1}{\Delta^2}+\frac{3}{2\Delta^4}\right]\right]\right\}\,,\end{aligned} \tag{3.21}$$

where

$$\alpha=1+\Delta^2\ . \tag{3.22}$$

In a similar manner we obtain the inelastic exchange-scattering amplitude for the $1s$-$3s$ transition:

$$\begin{aligned}T^{\rm ex}_{1s\text{-}3s}&=\frac{1}{3\sqrt{3}}\frac{4}{\pi^4}\left[1+\frac{2}{3}\frac{\partial}{\partial\lambda_2}+\frac{2}{27}\frac{\partial^2}{\partial\lambda_2^2}\right]\bar{A}\Big|_{\lambda_1=1,\ \lambda_2=1/3}\\
&=-\frac{8}{3\sqrt{3}\pi^2}\left\{\left[\frac{1}{\beta_0}\frac{27}{32}\left[-\frac{3}{2\alpha_0^2}+\frac{5}{2\alpha_0^3}-\frac{1}{\alpha_0^4}\right]+\frac{1}{\beta_0^2}\frac{3}{8}\left[\frac{9}{2\Delta_0^2}-\frac{9}{2\alpha_0}+\frac{7}{2\alpha_0^2}-\frac{1}{\alpha_0^3}\right]\right.\right.\\
&\quad+\frac{1}{\beta_0^3}\frac{1}{2}\left[-\frac{15}{4\Delta_0^2}+\frac{1}{\Delta_0^4}+\frac{9}{4\alpha_0}-\frac{3}{8\alpha_0^2}\right]+\frac{1}{\beta_0^4}\frac{1}{8}\left[\frac{11}{3\Delta_0^2}-\frac{29}{9\Delta_0^4}-\frac{5}{6\Delta_0^6}-\frac{1}{\alpha_0}\right]\\
&\quad+\frac{1}{2\beta_0^5}\frac{1}{81}\left[-\frac{5}{\Delta_0^2}+\frac{23}{6\Delta_0^4}-\frac{175}{48\Delta_0^6}-\frac{35}{16\Delta_0^8}\right]\Bigg]\\
&\quad+\frac{D_{13}}{\Delta_0}\left[\frac{1}{\beta_0^2}\left[\frac{27}{16\Delta_0^2}\right]+\frac{1}{4\beta_0^3}\left[3-\frac{31}{4\Delta_0^2}+\frac{9}{4\Delta_0^4}\right]+\frac{1}{3\beta_0^4}\left[-\frac{1}{3}+\frac{11}{8\Delta_0^2}-\frac{19}{12\Delta_0^4}-\frac{25}{96\Delta_0^6}\right]\right.\\
&\quad\left.\left.+\frac{1}{54\beta_0^5}\left[-\frac{5}{3}-\frac{17}{12\Delta_0^2}+\frac{5}{4\Delta_0^4}-\frac{95}{48\Delta_0^6}-\frac{35}{48\Delta_0^8}\right]\right]\right\}\,,\end{aligned} \tag{3.23}$$

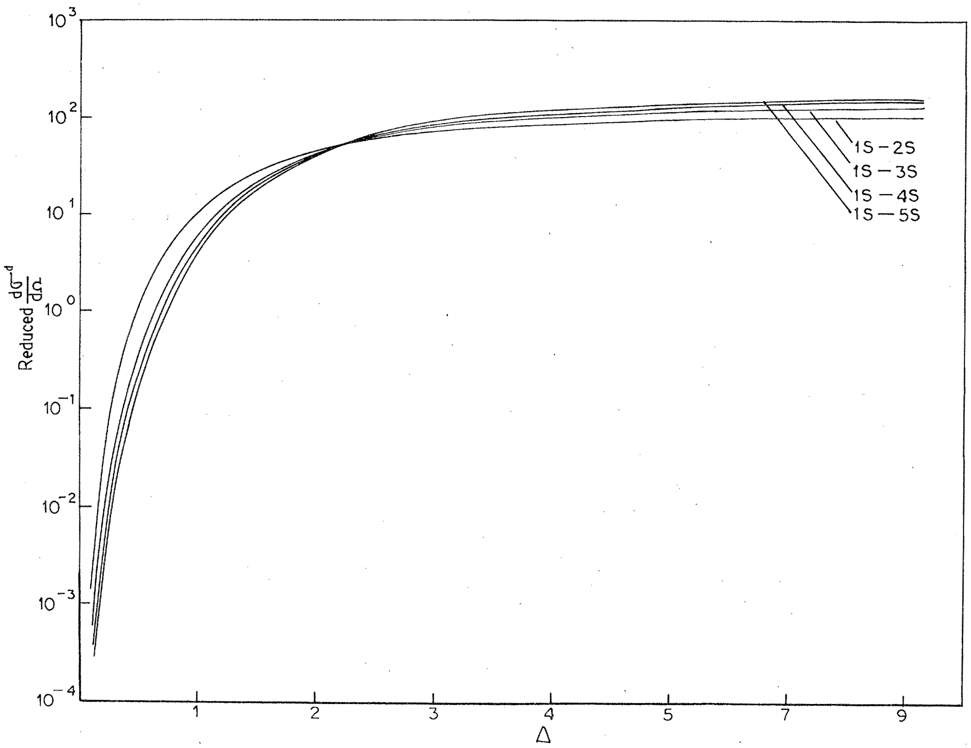

FIG. 1. Reduced direct differential cross section $d\sigma^d/d\Omega=[(n_1n_2)^3/g_1^2]\Delta^4 d\sigma^d/d\Omega$ for excitation of the n_2s ($n_s=2$–5) state of hydrogen from the ground state ($n_1=1$) by electron impact, plotted as a function of momentum transfer Δ at 300 eV incident electron energy.

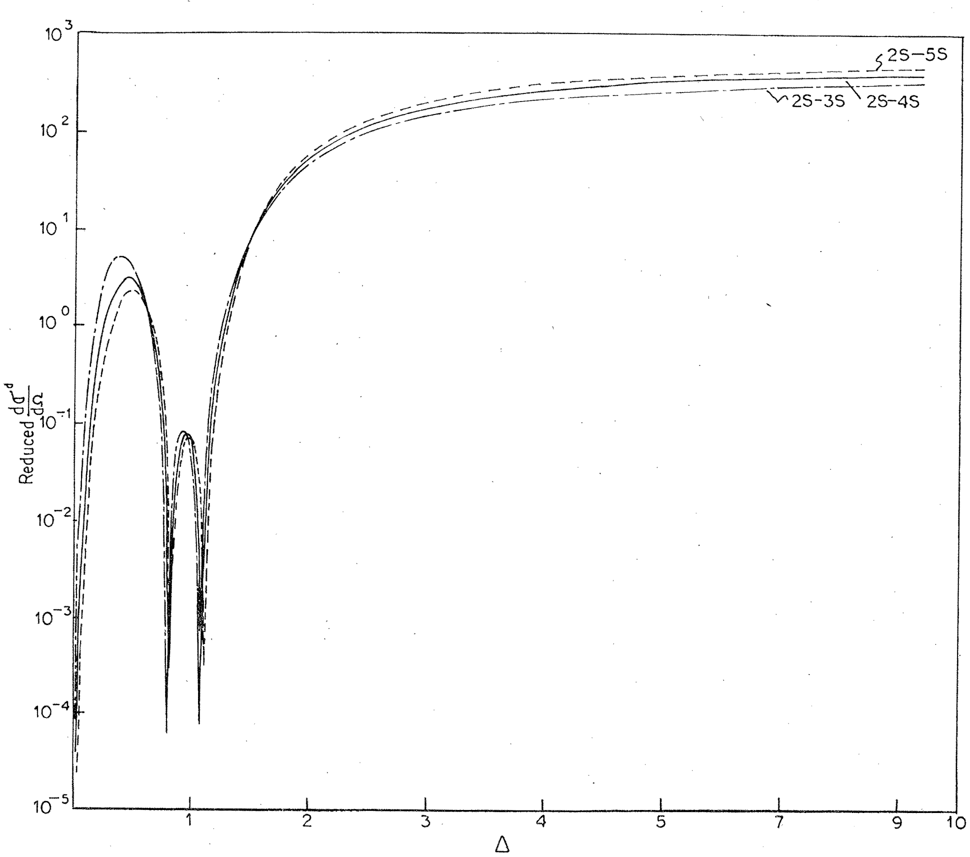

FIG. 2. Reduced $d\sigma^d/d\Omega$ vs Δ in the case of $2s$-n_2s ($n_2=3$–5) transition for 300 eV incident electron energy.

where

$$\Delta_0^2=(1+\tfrac{1}{3})^{-2}\Delta^2 , \quad (3.24)$$

$$\alpha_0=1+\Delta_0^2 . \quad (3.25)$$

The expressions D_{22} and D_{13} occurring in (3.21) and (3.23) are obtained from that of $D_{n_1n_2}$ [see (3.11)] by setting $\lambda_1=\lambda_2=\frac{1}{2}$ and $\lambda_1=1$, $\lambda_2=\frac{1}{3}$, respectively.

IV. NUMERICAL RESULTS AND DISCUSSIONS

It is evident from (2.13) that direct-scattering amplitude $T^d_{n_1s\text{-}n_2s}$ multiplied by the factor $(n_1n_2)^{3/2}(\Delta^2/g_1)$ and $g_1=-2\lambda/(\Delta^2+\lambda^2)^2$ tends to a constant value when momentum transfer Δ becomes extremely large in the case of electron—hydrogen-atom collisions. In Figs. 1—3 we plot the reduced $d\sigma^d/d\Omega=(n_1n_2)^3(\Delta^4/g_1^2)d\sigma^d/d\Omega$ for direct scattering in electron-hydrogen collisions. These reduced differential cross sections are represented graphically as a function of Δ for $1s$-ns ($n=2$—5) and $2s$-ns ($n=3$—5) transitions in Figs. 1 and 2, respectively. It appears from these diagrams that the number of maxima (or minima) depends upon the initial-state quantum number and is rather independent of final-state quantum number.

In Fig. 3 we plot the reduced $d\sigma/d\Omega$ versus Δ for the transition $9s$-$10s$ (involving large quantum numbers) using the general formula (2.13) for $T^d_{n_1s\text{-}n_2s}$. In Fig. 3 and also in Fig. 4, which involves infinitely large quantum numbers characterizing the transition, we find the presence of two series of maxima. The height of certain maximum of one series (called the first series) is always less than that of the adjacent maximum belonging to the other series (called the second series).

In Fig. 4 we plot reduced $d\sigma^d/d\Omega=\frac{1}{16}(n_1n_2)^3\Delta^8 d\sigma^d/d\Omega$ versus $1/\Delta$ for the transition n_1s-n_2s when both n_1 and n_2 are infinitely large using the formula (2.22) given in the form of a single integral over finite real domain, which is valid except when Δ is very small. Now the simplified formula (2.23) is equivalent to the above-mentioned formula defined by (2.22). The first term in the square brackets of (2.23) for $T^d_{n_1s\text{-}n_2s}$, $\sin^2(4/\Delta)$, is an oscillating quantity having positive sign and the remaining portion (expression as the difference of two quantities) in the square brackets is of opposite sign and of magnitude less than 1 if Δ is not too small. In the above case minima and maxima of $T_{n_1s\text{-}n_2s}$ are of opposite sign. As a consequence of this fact the minima (or maxima) of $T^d_{n_1s\text{-}n_2s}$ lead to the first series (or the second series) of

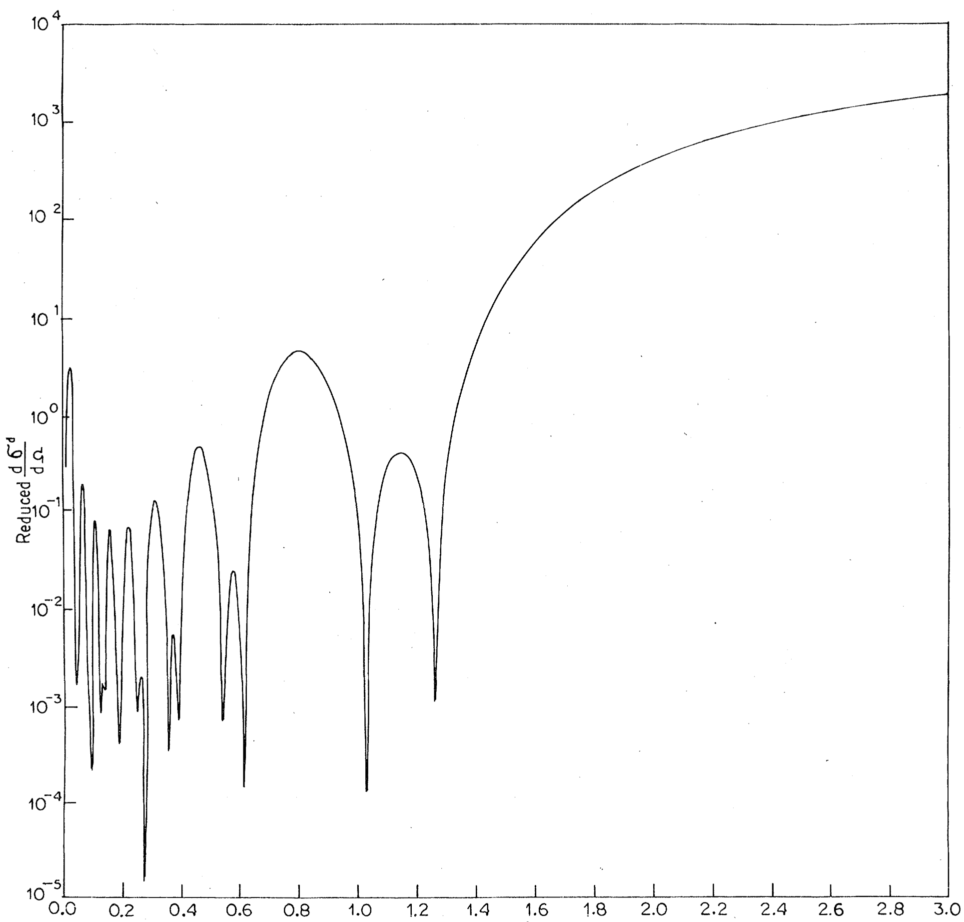

FIG. 3. Reduced direct differential cross section defined as in Fig. 1 for the $9s$-$10s$ transition as a function of momentum transfer Δ at 300 eV incident electron energy.

maxima of $d\sigma/d\Omega$ related to square of $T^{d}_{n_1s\text{-}n_2s}$. Keeping in mind the above discussion we find from (2.23) and Fig. 4 that the reduced $d\sigma^d/d\Omega$ monotonously decreases beyond $\Delta = 8/\pi$ and there is no maximum belonging to the first series beyond $\Delta = \Delta' = 4/\pi$. From (2.23) we further find that the maxima are equally spaced when plotted against $1/\Delta$. The spacing between one maximum (belonging to the first series) and the adjacent maximum (belonging to the second series) is $\pi/8$, when the differential cross section is plotted against $1/\Delta$. The above feature of equal spacing holds quite well in the case of Fig. 4 and also approximately in the case of Fig. 3. This spacing between two adjacent maxima is 0.392 829 and 0.4352 in Figs. 4 and 3, respectively, compared to the above theoretical value $\pi/8 = 0.392\,699$. The position of the last maximum of the first series with respect to Δ is at $\Delta' = 1.144\,763$ and 1.144 732 in Figs. 4 and 3, respectively, where the corresponding theoretical values of Δ is $\Delta' = 4/\pi = 1.273\,239$.

A study of the relations (2.13) and (3.10) shows that Δ^2 times the term of $O(1/\beta_0)$ of exchange-scattering amplitude is "equal" to β_0 $(=k_1^2+\lambda_2^2=k_2^2+\lambda_1^2)$ times the direct-scattering amplitude for the transition $n_1s\text{-}n_2s$ $(n_1 \neq n_2)$. The term of $O(1/\beta_0)$ corresponds to the Ochkur approximation. The above "equality" does not hold in the case of elastic scattering due to the presence of the term involving $\delta_{n_1n_2}$ in (2.13). In Fig. 5 we display two curves, one showing the variation of Δ^4 times the elastic direct differential cross section with change in Δ

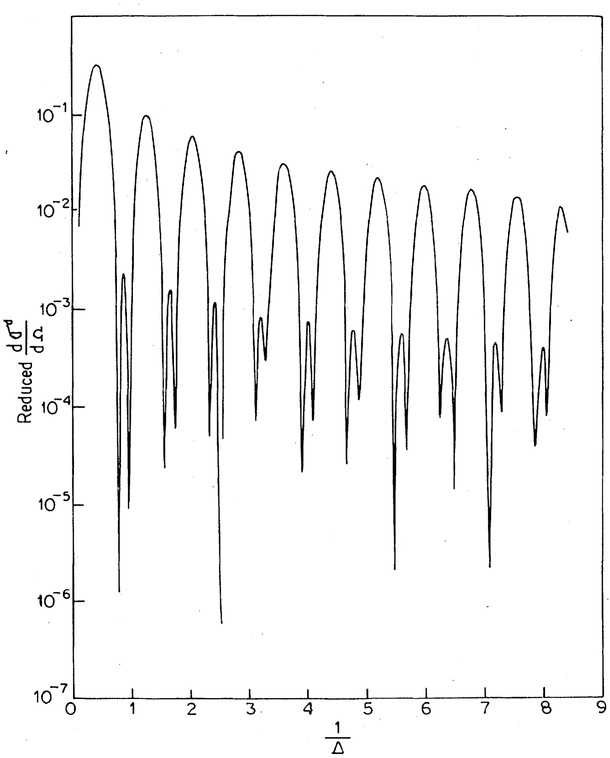

FIG. 4. Reduced direct differential cross section defined by $\frac{1}{16}(n_1n_2)^3\Delta^8 d\sigma^d/d\Omega$ [equal to the square of the integral occurring in (2.22)] plotted as a function of $1/\Delta$ for the $n_1s\text{-}n_2s$ transition where both n_1 and n_2 are extremely large in the case of electron-hydrogen collision at 300 eV incident electron energy.

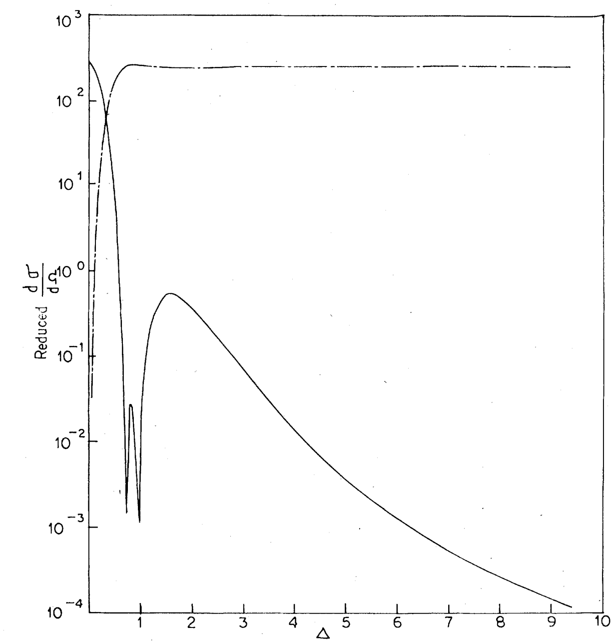

FIG. 5. Reduced differential cross section for 2*s*-2*s* elastic scattering of electrons by atomic hydrogen as a function of momentum transfer Δ at 300 eV incident electron energy. —·—, the variation of $\Delta^4(n_1n_2)^3$ times elastic direct differential cross section with change in Δ; ——, the dependence of $\beta_0^2(n_1,n_2)^3$ times exchange differential cross section on Δ.

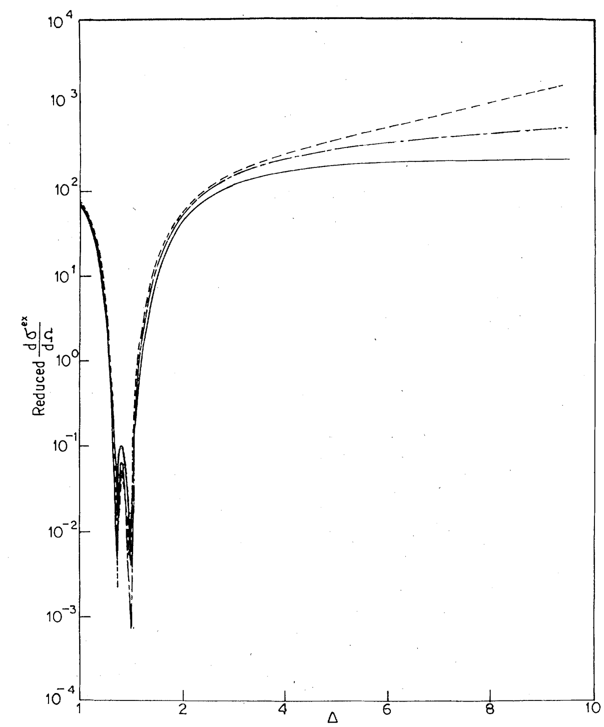

FIG. 6. Reduced exchange differential cross section $d\sigma^{ex}/d\Omega = [(n_1n_2)^3/g_1^2]\beta_0^2 d\sigma^{ex}/d\Omega$ for 2*s*-2*s* elastic exchange scattering of electrons by H atoms as a function of momentum transfer Δ at 300 eV incident electron energy for the following cases. ——, considering term of $O(1/\beta_0)$ in the exchange-scattering amplitude; —·—, for terms of $O(1/\beta_0)$ and $O(1/\beta_0^2)$ in the exchange-scattering amplitude; — — —, calculated from Eq. (3.21) which incorporates terms of all possible order in $1/\beta_0$.

and the other showing the dependence of β_0^2 times exchange differential cross section on Δ in the case of the $2s$-$2s$ transition. In Fig. 6 we have plotted reduced exchange differential cross section versus Δ using the expression given by (i) the particular relation (3.21) for $2s$-$2s$ transition consisting of terms of all possible order in powers of $1/\beta_0$, (ii) the term $O(1/\beta_0)$ of the general relation (3.10) corresponding to the Ochkur term, and (iii) the full general relation (3.10) consisting of terms of $O(1/\beta_0)$ and $O(1/\beta_0^2)$. In the case of Fig. 6 the reduced $d\sigma^{ex}/d\Omega$ is defined as $(n_1 n_2)^3(\beta_0^2/g_1^2)d\sigma^{ex}/d\Omega$. As is evident from Fig. 6, the correction to the Ochkur term is quite appreciable as Δ increases.

In all cases considered in this paper incident electron energy is taken to be 300 eV. The physical quantities appearing in this paper are expressed in atomic units.

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