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Perturbation Calculation of the Elastic Scattering of Electrons by Hydrogen Atoms*

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A perturbation calculation has been carried out for the scattering of electrons by hydrogen atoms, using as the perturbation only the interaction between the two electrons, and retaining in the result only terms of the highest power in the incident energy of the electron. The results are then compared with more conventional first-order perturbation calculations for this problem. It is found that to the order in the energy that we retain, the results for direct-scattered amplitudes obtained by the two perturbation procedures are the same, whereas in the results for the exchange-scattered amplitudes there is a difference in the energy dependence. While no conclusions can be drawn as to which perturbation procedure is more accurate, some reasons are given for preferring the calculation performed here.

1. INTRODUCTION

THE customary method[1] for treating the scattering of electrons by hydrogen atoms in the Born approximation is to take as the perturbation the interaction of the incoming electron with both particles of the atom, and to take matrix elements of this perturbation between initial and final states of the system. We shall call this the method of the "asymmetric perturbation," since it is not symmetric in the two electrons.

If the mass of the proton is taken to be infinite, one can, as an alternative, take as the perturbation simply the interaction between the two electrons. (This we call the "symmetric perturbation.") In this case the unperturbed Hamiltonian is separable, and the initial and final state wave functions corresponding to it can be exhibited in closed form.

This latter procedure is likely to lead to more accurate results than the former, since we include more of the interaction in our unperturbed problem. This advantage will be most pronounced in the calculation of exchange scattering. In this case the approximation with the asymmetric perturbation seems to be particularly poor since it leads to the physically absurd result that exchange scattering will occur even when the interaction between the two electrons vanishes.

In this paper we shall calculate separately the direct and the elastic exchange-scattered amplitude in the first Born approximation, taking as the perturbation the interaction between the two electrons. These two amplitudes can then be combined[1] to give the total differential cross section. We will consider energies high enough so that the term we calculate is likely to be the first of a convergent series, yet not so large that we need include relativistic effects. Since the energies we consider will be high, we will compute only the dependence of the result on the highest power of the energy.

As our results will show, the direct-scattered amplitude is the same, to the highest power in the energy, whether one uses the symmetric or asymmetric perturbation. For the exchange-scattered amplitude, on the other hand, the energy dependence at high energies in our results differs from that obtained by the method of asymmetric perturbation. Recalling the unphysical nature of the expression for the exchange-scattered amplitude when the asymmetric perturbation is used, we may presume that this amplitude is given more correctly by our calculation.

After some preliminary remarks in Sec. 2 which establish the integrals which must be evaluated, we calculate, in Sec. 3, the elastic direct-scattered amplitude and the elastic exchange-scattered amplitude. In Sec. 4 we discuss the results and compare them with the results of a similar calculation done with the asymmetric perturbation. The Appendix is devoted to a detailed evaluation of a typical integral occurring in Sec. 3.

2. PRELIMINARY CONSIDERATIONS

In order to calculate the elastic-scattered amplitudes, we take the mass of the proton to be infinite and seek a solution of the Schrödinger equation for the system

$$\left\{\Delta_1+\Delta_2+2\left(E+\frac{1}{r_1}+\frac{1}{r_2}-\frac{1}{r_{12}}\right)\right\}\Psi=0, \quad (2.1)$$

which represents an incoming plane wave in electron 1 and outgoing spherical waves in particles 1 or 2 as r_1 or $r_2\rightarrow\infty$. We are using a system of units in which $m=\hbar=e=1$. The unit of length is thus the Bohr radius, and the unit of energy is 27.06 ev, that is, twice the ionization energy of hydrogen. The outgoing spherical waves each correspond to one of the energies allowed by the conservation of energy. When we confine ourselves to elastic scattering, as we do in this paper, we seek the coefficients f_0 and g_0 of the outgoing spherical waves as r_1 and r_2, respectively, approach infinity. These are the coefficients of the spherical waves having the same energy as the incoming particle.

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[1] N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949), second edition, Chap. VIII.

The expression for the exchange-scattered amplitude in first-order perturbation is given by

$$g_0=-\frac{1}{2\pi}\int\Psi_f^*V\Psi_i d\tau_1 d\tau_2, \tag{2.2}$$

where V is the perturbation. When we choose the asymmetric perturbation

$$V=2(1/r_1-1/r_{12}), \tag{2.3}$$

then the exchange-scattered amplitude is

$$g_{0a}=-\frac{1}{\pi^2}\int \exp(-r_1-i\mathbf{k}_n\cdot\mathbf{r}_2+i\mathbf{k}_0\cdot\mathbf{r}_1)\times\left[\frac{1}{r_1}-\frac{1}{r_{12}}\right]d\tau_1 d\tau_2, \tag{2.4}$$

where $\mathbf{k}_0$, $\mathbf{k}_n$ are the propagation vectors of the electrons in the initial and final states.

In the case of the exchange-scattered amplitude in Eq. (2.4), there is some question as to whether the perturbation V should be $2(1/r_1-1/r_{12})$ or $2(1/r_2-1/r_{12})$. If, as in this case, one knows the bound-state wave functions exactly, either perturbation yields the same result;[2] however, in problems involving more complicated atoms whose wave functions are not known precisely, this freedom of choice is the origin of the post-prior discrepancy.[3]

If one chooses the symmetric perturbation

$$V=2/r_{12}, \tag{2.5}$$

then the exchange-scattered amplitude is given by

$$\begin{aligned}g_{0s}=\frac{N^2}{\pi^2}\int &\exp(-r_1+i\mathbf{k}_0\cdot\mathbf{r}_1-r_2-i\mathbf{k}_n\cdot\mathbf{r}_2)\frac{1}{r_{12}}\\ &\times{}_1F_1(-i/k,1,i(kr_2+\mathbf{k}_n\cdot\mathbf{r}_2))\\ &\times{}_1F_1(-i/k,1,i(kr_1-\mathbf{k}_0\cdot\mathbf{r}_1))d\tau_1 d\tau_2,\end{aligned} \tag{2.6}$$

where $k=|\mathbf{k}_0|=|\mathbf{k}_n|$, and $k^2=2(E+\frac{1}{2})$; furthermore,

$$N^2=\frac{(\pi/k)\exp(-\pi/k)}{\sinh(\pi/k)} \tag{2.7}$$

is the normalization constant for the continuum hydrogen functions corresponding to incident waves of unit amplitude. The ${}_1F_1$ are confluent hypergeometric functions.

The direct-scattered amplitude when the asymmetric perturbation in Eq. (2.3) is used can also be obtained from Eq. (2.2); we have

$$f_{0a}=-\frac{1}{\pi^2}\int\exp[-2r_2+i(\mathbf{k}_0-\mathbf{k}_n)\cdot\mathbf{r}_1]\times\left(\frac{1}{r_1}-\frac{1}{r_{12}}\right)d\tau_1 d\tau_2. \tag{2.8}$$

If, however, we use the symmetric perturbation of Eq. (2.5), we must add the Rutherford scattering amplitude to the amplitude corresponding to Eq. (2.2). This additional term arises from the circumstance that our unperturbed problem contains an outgoing wave as $r_1\to\infty$.[4] For the symmetric perturbation we have, then,[5]

$$\begin{aligned}f_{0s}=\frac{N^2}{\pi^2}\int&\exp[-2r_2+i(\mathbf{k}_0-\mathbf{k}_n)\cdot\mathbf{r}_1]\\ &\times{}_1F_1(-i/k,1,i(kr_1+\mathbf{k}_n\cdot\mathbf{r}_1))\frac{1}{r_{12}}\\ &\times{}_1F_1(-i/k,1,i(kr_1-\mathbf{k}_0\cdot\mathbf{r}_1))d\tau_1 d\tau_2+R,\end{aligned} \tag{2.9}$$

where

$$R=\frac{[2ikr\sin^2(\theta/2)]^{i/k}}{[-2ikr\sin^2(\theta/2)]^{-i/k}}\frac{\Gamma(1-i/k)}{\Gamma(1+i/k)}\frac{1}{k^2}\frac{1}{\sin^2(\theta/2)}; \tag{2.10}$$

here Γ is the gamma function of its argument.

The calculation of Eqs. (2.9) and (2.6) will give respectively the direct- and exchange-scattered amplitudes in our approximation. These will be compared with the results obtained from Eqs. (2.8) and (2.4) which have been computed by Corinaldesi and Trainor.[6]

3. DIRECT SCATTERING

The integration of (2.9) with respect to the $\mathbf{r}_2$ coordinate can be done immediately, and yields

$$\begin{aligned}f_{0s}=\frac{N^2}{\pi}\int\Big\{&\exp[-2r_1+i(\mathbf{k}_0-\mathbf{k}_n)\cdot\mathbf{r}_1]\\ &\times{}_1F_1(-i/k,1,i(kr_1+\mathbf{k}_n\cdot\mathbf{r}_1))\\ &\times\left[1+\frac{1}{r_1}\right]{}_1F_1(-i/k,1,i(kr_1-\mathbf{k}_0\cdot\mathbf{r}_1))\Big\}d\tau_1\\ +\frac{N^2}{\pi}\int\Big\{&\exp[i(\mathbf{k}_0-\mathbf{k}_n)\cdot\mathbf{r}_1]\\ &\times{}_1F_1(-i/k,1,i(kr_1+\mathbf{k}_n\cdot\mathbf{r}_1))\frac{1}{r_1}\\ &\times{}_1F_1(-i/k,1,i(kr_1-\mathbf{k}_0\cdot\mathbf{r}_1))\Big\}d\tau_1+R.\end{aligned} \tag{3.1}$$

The second and third terms of Eq. (3.1) may be considered in a different context. Suppose one considered the scattering of an electron by a positive and negative charge of the same magnitude situated at the same point in space. If now one evaluates the scattered amplitude in first Born approximation, using as the unperturbed problem the potential due to the positive charge alone, then the result is just the sum of the

[2] S. Altshuler, Phys. Rev. **91**, 1167 (1953).

[3] D. R. Bates *et al.*, Trans. Roy. Soc. (London) **A243**, 93 (1950).

[4] S. Borowitz and B. Friedman, Phys. Rev. **89**, 441 (1953).

[5] A. Sommerfeld, *Wellenmechanik* (Frederich Ungar Publishing Company, New York, 1939), p. 502; H. A. Bethe and G. Breit, Phys. Rev. **93**, 888 (1954).

[6] A. Corinaldesi and P. Trainor, Nuovo cimento **2**, 940 (1952).

second and third terms of Eq. (3.1). This sum is not zero, due to the crudity of the first Born approximation.[7] Obviously, however, the scattering due to this configuration, if calculated exactly, would vanish. Therefore we feel justified in considering the second term in Eq. (3.1) as cancelled by the third.

The first term of Eq. (3.1) then gives us the symmetric-scattered amplitude. We write this as

$$f_{0s}=-(N^2/\pi)(I_0+I_1), \tag{3.2}$$

where

$$I_0=\int \exp[-\lambda r+i(\mathbf{k}_0-\mathbf{k}_n)\cdot\mathbf{r}] \times {}_1F_1(-i/k,1,i(kr+\mathbf{k}_n\cdot\mathbf{r})) \times {}_1F_1(-i/k,1,i(kr-\mathbf{k}_0\cdot\mathbf{r}))\frac{d\tau}{r}\bigg|_{\lambda=2}, \tag{3.3}$$

and

$$I_1=-\partial I_0/\partial\lambda|_{\lambda=2}. \tag{3.4}$$

Using a method introduced by Sommerfeld,[8] we have computed the integral I_0; the result is

$$I_0=\frac{4\pi}{4k^2\sin^2(\theta/2)+\lambda^2}e^{\pi/k}\left[\frac{4(k+\frac{1}{2}i\lambda)^2}{4k^2\sin^2(\theta/2)+\lambda^2}\right]^{i/k} \times {}_2F_1\left(1+i/k,-i/k,1,1-\frac{\lambda^2}{4k^2\sin^2(\theta/2)+\lambda^2}\right)\bigg|_{\lambda=2}, \tag{3.5}$$

where ${}_2F_1$ is the hypergeometric function of its argument.

From Eqs. (3.4) and (3.5) one could calculate f_{0s} exactly; but we are interested only in the highest power of k in f_{0s}. To find this we first investigate the highest power of k in I_0. This involves the reduction of the hypergeometric function ${}_2F_1$. We set

$$\frac{\lambda^2}{4k^2\sin^2(\theta/2)+\lambda^2}=\epsilon; \tag{3.6}$$

then we have

$${}_2F_1(1+i/k,-i/k,1,1-\epsilon) =\frac{1}{\Gamma(1+i/k)\Gamma(-i/k)}\sum_{n=0}^{\infty}\frac{(1+i/k)_n(-i/k)_n}{n!n!} \times[2\Psi(1+n)-\Psi(1+i/k+n)+\Psi(-i/k+n)-\log\epsilon]\epsilon^n, \tag{3.7}$$

(Erdelyi,[9] p. 112, formula 14 with $m=0$). Here $\Psi(x)=\Gamma'(x)/\Gamma(x)$. To the highest power of k,

$${}_2F_1(1+i/k,-i/k,1,1-\epsilon)\cong\frac{1}{\Gamma(1+i/k)\Gamma(-i/k)} \times[-2\gamma+\Psi(-i/k)\Psi(1+i/k)], \tag{3.8}$$

where γ = Euler's constant $=0.577215\cdots$. But

$$\Gamma(1+i/k)\Gamma(-i/k)=\frac{\pi i}{\sinh(\pi/k)} \tag{3.9}$$

(Erdelyi,[9] p. 3), and

$$\Psi(-i/k)-\Psi(1+i/k)=(\pi/i)\coth(\pi/k) \tag{3.10}$$

(Erdelyi,[9] p. 15). Consequently,

$${}_2F_1(1+i/k,1,1-\epsilon) \cong\frac{\sinh(\pi/k)}{\pi i}\left[-\gamma+\frac{\pi}{i}\coth(\pi/k)-\log\epsilon\right] \cong-\cosh(\pi/k)\cong-1 \tag{3.11}$$

to the highest power of k.

The contribution of I_1 can be evaluated from Eq. (3.4). Differentiating the coefficient of the hypergeometric function gives terms of lower order in k than those we have considered. Hence we must differentiate the hypergeometric function. We obtain

$$I_1\cong-\frac{4\pi}{4k^2\sin^2(\theta/2)+\lambda^2}e^{\pi/k}\left[\frac{4(k+\frac{1}{2}i\lambda)^2}{4k^2\sin^2(\theta/2)+\lambda^2}\right]^{i/k} \times\frac{d}{d\lambda}\left[{}_2F_1\left(1+\frac{i}{k},-\frac{i}{k},1,1-\frac{\lambda^2}{4k^2\sin^2(\theta/2)+\lambda^2}\right)\right]\bigg|_{\lambda=2}$$
$$=-\frac{4\pi}{4k^2\sin^2(\theta/2)+\lambda^2}e^{\pi/k}\left[\frac{4(k+\frac{1}{2}i\lambda)^2}{4k^2\sin^2(\theta/2)+\lambda^2}\right]^{i/k} \times\left(1+\frac{i}{k}\right)\left(-\frac{i}{k}\right){}_2F_1\left(2+\frac{i}{k},1-\frac{i}{k},2,1-\frac{\lambda^2}{4k^2\sin^2(\theta/2)+\lambda^2}\right)-\frac{8\lambda k^2\sin^2(\theta/2)}{[4k^2\sin^2(\theta/2)+\lambda^2]^2} \tag{3.12}$$

(Erdelyi,[9] p. 102). But

$${}_2F_1(2+i/k,1-i/k,2,1-\epsilon) =\frac{1}{\epsilon\Gamma(2+i/k)\Gamma(1-i/k)}+\frac{(-1)^n}{(1+i/k)(-i/k)} \times\sum_{n=0}^{\infty}\frac{(2+i/k)_n(1-i/k)_n}{(n+1)!n!}[\Psi(1+n)+\Psi(2+n)-\Psi(2+i/k+n)+\Psi(1-i/k+n)-\log\epsilon]\epsilon^n \tag{3.13}$$

[7] I am indebted to Professor Zumino for this remark. A direct calculation of the second term of Eq. (3.1) gives an infinite result when $|k_0|=|k_n|$. This is related to the fact that plane waves cannot be generated by iterating with hydrogenic wave functions.

[8] A. Sommerfeld, reference 5, pp. 503–506. A. Nordsieck [Phys. Rev. **93**, 785 (1954)] has also computed the integral I_0 and obtained the same result as we did. Nordsieck has confined himself to the case where λ is small. However, his result can be shown to be valid for all positive λ.

[9] Erdelyi, Magnus, Oberhettinger, and Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, New York, 1953), Vol. 1.

(Erdelyi,[9] p. 110). Now we restrict ourselves to the highest power of k, and use Eq. (3.9) and the fact that

$$\Psi(1-i/k)-\Psi(1+i/k)=-\frac{1}{i/k}+\pi\cot(\pi i/k) \quad (3.14)$$

(Erdelyi,[9] p. 16) to obtain

$${}_2F_1(2+i/k,\,1-i/k,\,2,\,1-\epsilon)\cong 2. \quad (3.15)$$

Thus the contribution of I_1 to f_0 is of the order of $1/k^3$ with respect to the I_0. To find the contribution of I_0 to f_0, we substitute Eq. (3.11) into Eq. (3.5), and substitute the result into Eq. (3.2); using Eq. (2.7) we obtain

$$f_0=-\frac{1}{k^2\sin^2(\theta/2)+1}, \quad (3.16)$$

to the highest power in k. This is precisely the result to the highest power in k which is obtained when one uses the asymmetric perturbation.[6]

4. EXCHANGE SCATTERING

The exchange-scattered amplitude in first-order perturbation theory, with $1/r_{12}$ as the perturbation, is given by Eq. (2.6). In order to evaluate this integral we first introduce the Fourier transform,

$$\frac{1}{r_{12}}=\frac{1}{2\pi^2}\int\frac{\exp[i\mathbf{K}\cdot(\mathbf{r}_1-\mathbf{r}_2)]}{K^2-i\epsilon}d\mathbf{K}. \quad (4.1)$$

[In what follows we will omit explicit mention of the ϵ in Eq. (4.1).] Equation (2.6), then, becomes

$$g_0=-\frac{N^2}{2\pi^4}\int\exp[-r_1+i(\mathbf{K}-\mathbf{k}_n)\cdot\mathbf{r}_1-r_2-i(\mathbf{K}-\mathbf{k}_0)\cdot\mathbf{r}_2]$$
$$\times{}_1F_1(-i/k,\,1,\,i(kr_2-\mathbf{k}_0\cdot\mathbf{r}_2))$$
$$\times{}_1F_1(-i/k,\,1,\,i(kr_1+\mathbf{k}_n\cdot\mathbf{r}_1))\frac{d\mathbf{K}}{K^2}d\tau_1 d\tau_2. \quad (4.2)$$

Equation (4.2) can now be separated into a product of functions of r_1 and r_2:

$$g_0=-\frac{N^2}{2\pi^4}\int J_1'(\mathbf{K})J_2'(\mathbf{K})\frac{d\mathbf{K}}{K^2}, \quad (4.3)$$

where

$$J_1'(\mathbf{K})=\int\exp[-r_1+i(\mathbf{K}-\mathbf{k}_n)\cdot\mathbf{r}_1]$$
$$\times{}_1F_1(-i/k,\,1,\,i(kr_1+\mathbf{k}_n\cdot\mathbf{r}_1))d\tau_1, \quad (4.4)$$

$$J_2'(\mathbf{K})=\int\exp[-r_2-i(\mathbf{K}-\mathbf{k}_0)\cdot\mathbf{r}_2]$$
$$\times{}_1F_1(-i/k,\,1,\,i(kr-\mathbf{k}_0\cdot\mathbf{r}_2))d\tau_2. \quad (4.5)$$

Instead of evaluating Eq. (4.4) directly, it is simpler to evaluate the integral

$$J_1(\alpha,\mathbf{K})=\int\exp[-\alpha r_1+i(\mathbf{K}-\mathbf{k}_n)\cdot\mathbf{r}_1]$$
$$\times{}_1F_1(-i/k,\,1,\,i(kr_1+\mathbf{k}_n\cdot\mathbf{r}_1))r_1dr_1d\Omega_1d\phi, \quad (4.6)$$

which is related to J_1' by

$$J_1'=-\partial J_1/\partial\alpha|_{\alpha=1}. \quad (4.7)$$

We may proceed similarly for Eq. (4.5). Then we obtain

$$g_{0s}=-\frac{N^2}{2\pi^4}\int\frac{\partial^2}{\partial\alpha\partial\beta}J_1(\alpha,\mathbf{K})J_2(\beta,\mathbf{K})\frac{d\mathbf{K}}{K^2}. \quad (4.8)$$

The difficulty in evaluating the integrals corresponding to J_1 and J_2 lies in the fact that two distinct and variable angles are involved, namely the angles between $(\mathbf{K}-\mathbf{k}_n)$ and $\mathbf{r}$ and between $\mathbf{k}_n$ and $\mathbf{r}$. We can circumvent this difficulty by using an integral representation[10] for the confluent hypergeometric function. This yields

$$J_1=\frac{1}{2\pi i}\oint\left(\frac{u}{u+1}\right)^{i/k}\frac{1}{u}\exp\{-r(\alpha+iku)$$
$$+i[\mathbf{K}-\mathbf{k}_n(1+u)]\cdot\mathbf{r}\}rdrd\Omega du, \quad (4.9)$$

where the integration in u space is a path surrounding the points 0 and -1. The space integrals of Eq. (3.1) are now readily evaluated to give

$$J_1=\frac{1}{2\pi i}\oint\left(\frac{u}{u+1}\right)^{i/k}\frac{1}{u}\frac{4\pi}{(\alpha+iku)^2+[\mathbf{K}-\mathbf{k}_n(1+u)]^2}du,$$
$$=\frac{1}{2\pi i}\oint\left(\frac{u}{u+1}\right)^{i/k}\frac{1}{u}\frac{4\pi}{\xi-\zeta u}du, \quad (4.10)$$

where

$$\xi=(\alpha^2+|\mathbf{K}-\mathbf{k}_n|^2),$$
$$\zeta=[2(\mathbf{K},\mathbf{k}_n)-k^2-i\alpha k]. \quad (4.11)$$

Now as $u\to\infty$ the integrand of Eq. (3.2) tends to zero as $1/u^2$. Since ξ/ζ does not lie on the real axis between -1 and 0, we may evaluate Eq. (4.10) by the residue theorem; we get

$$J_1=\frac{4\pi}{\xi}\left(\frac{\xi}{\xi+\zeta}\right)^{i/k}. \quad (4.12)$$

Since we wish to find $\partial J_1/\partial\alpha|_{\alpha=1}$ rather than J, we differentiate Eq. (4.12) with respect to α and set the derivative equal to 1. The result is

$$\left.\frac{\partial J_1}{\partial\alpha}\right|_{\alpha=1}=-\frac{16\pi}{(1+|\mathbf{K}-\mathbf{k}_n|^2)^2}$$
$$\times\left(\frac{K^2-(\mathbf{n},\mathbf{K})(k+i)}{K^2-(k+i)^2}\right)\left(\frac{\xi}{\xi+\zeta}\right)^{i/k}. \quad (4.13)$$

Here $\mathbf{n}$ is a unit vector in the direction of k_n. By a

[10] See A. Sommerfeld, reference 5, p. 461.

similar procedure we obtain

$$\left.\frac{\partial J_2}{\partial\beta}\right|_{\beta=1}=-\frac{16\pi}{(1+|\mathbf{K}-\mathbf{k}_0|^2)^2}\left(\frac{K^2-(\mathbf{n}_0,\mathbf{K})(k+i)}{[K^2-(k+i)^2]}\right)\left(\frac{\xi_0}{\xi_0+\zeta_0}\right)^{i/k}, \tag{4.14}$$

where ξ_0 and ζ_0 are related to $\mathbf{k}_0$ as ξ and ζ to $\mathbf{k}_n$.

Now using Eqs. (4.8), (4.13), and (4.14), we obtain

$$g_{0s}=-\frac{128N^2}{\pi^2}\cdot\int\frac{d\mathbf{K}}{K^2}\frac{K^4-K^2(k+i)[(\mathbf{n}_0,\mathbf{K})+(\mathbf{n},\mathbf{K})]+(k+i)^2[(\mathbf{n}_0,\mathbf{K})(\mathbf{n},\mathbf{K})]}{(1+|\mathbf{K}-\mathbf{k}_0|^2)^2(1+|\mathbf{K}-\mathbf{k}_n|^2)^2[K^2-(k+i)^2]^2}\left(\frac{\xi}{\xi+\zeta}\right)^{i/k}\left(\frac{\xi_0}{\xi_0+\zeta_0}\right)^{i/k}. \tag{4.15}$$

It is interesting to compare Eq. (4.15) with the corresponding term that would arise if one were to compute the matrix elements of $1/r_{12}$ using plane waves instead of hydrogenic continuum functions; this term is

$$g_{0p}=-\frac{32}{\pi^2}\int\frac{d\mathbf{K}}{K^2}\frac{1}{(1+|\mathbf{K}-\mathbf{k}_0|^2)^2}\frac{1}{(1+|\mathbf{K}-\mathbf{k}_n|^2)^2}. \tag{4.16}$$

The differences between Eqs. (4.16) and (4.15) which can be identified are: (i)—that Eq. (4.16) contains a normalization constant N^2, which tends to 1 as $k\rightarrow\infty$; (ii)—Eq. (4.15) contains an extra term $[K^2-(k+i)^2]^2$ in the denominator; this is the sort of term that would arise from the matrix element of $1/r_{12}$ between outgoing spherical waves of the form e^{ikr}/r; and (iii)—Eq. (4.15) contains the factors $[\xi/(\xi+\zeta)]^{i/k}$ and $[\xi_0/(\xi_0+\zeta_0)]^{i/k}$, which resemble terms that might come from a logarithmic phase factor at infinity in the asymptotic form of the continuum hydrogenic wave functions. We shall now show that if, as in the present study, we consider only the highest power in k in g_{0s}, we may replace the last two factors in Eq. (4.15) by unity. First we note that since the integral is absolutely convergent we may expand $[\xi/(\xi+\zeta)]^{i/k}$ and $[\xi_0/(\xi_0+\zeta_0)]^{i/k}$. The result of this expansion is $1+S$, where S is a complex number whose real part is $\leq\pi/k$ and whose imaginary part is $\leq(p/k)\log k$, with p finite. Since both these terms approach 0 as $k\rightarrow\infty$, we may neglect S in investigating the k-dependence of g_{0s} as $k\rightarrow\infty$.

Now, replacing $[\xi/(\xi+\zeta)]^{i/k}$ and $[\xi_0/(\xi_0+\zeta_0)]^{i/k}$ by 1 in Eq. (4.15), we have the approximate expression:

$$g_{0s}\cong-\frac{128N^2}{\pi^2}\int\frac{d\mathbf{K}}{K^2}\left(\frac{K^4-K^2(k+i)[(\mathbf{n}_0,\mathbf{K})+(\mathbf{n},\mathbf{K})]+(k+i)^2[(\mathbf{n}_0,\mathbf{K})(\mathbf{n},\mathbf{K})]}{(1+|\mathbf{K}-\mathbf{k}_0|^2)^2[K^2-(k+i)^2]^2(1+|\mathbf{K}-\mathbf{k}_n|^2)^2}\right), \tag{4.17}$$

which we shall now proceed to evaluate exactly. Equation (4.17) may be simplified somewhat and then written in the more tractable form

$$\begin{aligned}g_{0s}\cong-\frac{128N^2}{\pi^2}\int d\mathbf{K}&\frac{1}{[K^2-(k+i)^2](1+|\mathbf{K}-\mathbf{k}_0|^2)^2(1+|\mathbf{K}-\mathbf{k}_n|^2)^2}+\frac{(k+i)^2}{[K^2-(k+i)^2]^2(1+|\mathbf{K}-\mathbf{k}_0|^2)^2(1+|\mathbf{K}-\mathbf{k}_n|^2)^2}\\&-\frac{(k+i)[(\mathbf{n}_0,\mathbf{K})+(\mathbf{n},\mathbf{K})]}{[K^2-(k+i)^2]^2(1+|\mathbf{K}-\mathbf{k}_0|^2)^2(1+|\mathbf{K}-\mathbf{k}_n|^2)^2}+\frac{(k+i)^2(\mathbf{k}_0,\mathbf{K})(\mathbf{k},\mathbf{K})}{K^2[K^2-(k+i)^2]^2(1+|\mathbf{K}-\mathbf{k}_0|^2)^2(1+|\mathbf{K}-\mathbf{k}_n|^2)^2}.\end{aligned} \tag{4.18}$$

The four terms of Eq. (4.18) will henceforth be designated as integrals I, II, III, IV respectively. These integrals can be evaluated by the method developed by Feynman.[11] In this technique terms of the form $1/A_1\cdots A_n$ are replaced by integrals, as follows:

$$\frac{1}{A_1\cdots A_n}=(n-1)!\int\frac{\delta(x_1+x_2+\cdots x_{n-1})dx_1\cdots dx_n}{[Ax_1\cdots+A_nx_n]^n},\quad x_i\geq 0. \tag{4.19}$$

Our denominators in Eq. (4.18) do not occur to the first power, but can be put in the form (4.19) since

$$\frac{1}{A_1{}^s\cdots A_2\cdots A_n}=(-1)^{s-1}(n+s-1)!\int\frac{x_1{}^s\delta(x_1+x_2\cdots+x_n-1)dx_1\cdots dx_n}{[Ax_1+\cdots+A_nx_n]^{n+s}},\quad x_i\geq 0,\quad i=1,2,\cdots n. \tag{4.20}$$

Also, the terms in Eq. (4.18) containing $(\mathbf{n}_0,\mathbf{K})$ in the numerator can be put in the form (4.19) using the identity

$$\frac{(\mathbf{n}_0,\mathbf{K})}{[1+K^2-2(\mathbf{K},\mathbf{k}_0)+k^2]^2}=\frac{1}{2}\frac{\partial}{\partial k_0}\frac{1}{[1+K^2-2(\mathbf{K},\mathbf{k}_0)+k^2]}. \tag{4.21}$$

[11] R. P. Feynman, Phys. Rev. **76**, 769 (1949); R. Jost and A. Pais, Phys. Rev. **82**, 840 (1951).

Using Eqs. (4.20), (4.21), and (4.19), Eq. (4.18) becomes

$$\mathrm{I}=4!\int\frac{x_2x_3\delta(x_1+x_2+x_3-1)dx_1dx_2dx_3d\mathbf{K}}{\{[K^2-(k+i)^2]x_1+(|\mathbf{K}-\mathbf{k}_0|^2+1)x_2+(|\mathbf{K}-\mathbf{k}_n|^2+1)x_3\}^5},\tag{4.22}$$

$$\frac{\mathrm{II}}{(k+i)^2}=-5!\int\frac{x_1x_2x_3\delta(x_1+x_2+x_3-1)dx_1dx_2dx_3d\mathbf{K}}{\{[K^2-(k+i)^2]x_1+(|\mathbf{K}-\mathbf{k}_0|^2+1)x_2+(|\mathbf{K}-\mathbf{k}_n|^2+1)x_3\}^6},\tag{4.23}$$

$$\frac{\mathrm{III}}{(k+i)}=-\frac{1}{2}\frac{\partial}{\partial k_0}4!\int\frac{x_1x_3\delta(x_1+x_2+x_3-1)dx_1dx_2dx_3d\mathbf{K}}{\{[K^2-(k+i)^2]x_1+(1+K^2+k^2-2(\mathbf{K},\mathbf{k}_0))x_2+(1+|\mathbf{K}-\mathbf{k}_n|^2)x_3\}^5}$$
$$-\frac{1}{2}\frac{\partial}{\partial k_n}4!\int\frac{x_1x_2\delta(x_1+x_2+x_3-1)dx_1dx_2dx_3d\mathbf{K}}{\{[K^2-(k+i)^2]x_1+(1+|\mathbf{K}-\mathbf{k}_0|^2)x_2+[1+K^2+k^2-2(\mathbf{K},\mathbf{k}_n)]x_3\}^5},\tag{4.24}$$

$$\frac{\mathrm{IV}}{(k+i)^2}=-\frac{1}{4}\frac{\partial}{\partial k_0}\frac{\partial}{\partial k_n}4!\int\frac{x_4\delta(x_1+x_2+x_3+x_4-1)dx_1dx_2dx_3d\mathbf{K}}{\{K^2x_1+[1+K^2+k^2-2(\mathbf{K},\mathbf{k}_0)]x_2+[1+K^2+k^2-2(\mathbf{K},\mathbf{k}_n)]x_3+[K^2-(k+i)^2]x_4\}^5},$$
$$x_i\geq 0.\tag{4.25}$$

We now follow the Feynman technique exactly in evaluating Eqs. (4.22)–(4.25). As an example of the use of this method we have computed Eq. (4.24) in detail in Appendix I. The others are computed by a straightforward use of the same method. We obtain

$$\mathrm{I}=\frac{15\pi^2}{64}\frac{1}{(k^2\mu)^{7/2}}\int_0^1du\int_{-u}^{u}dv\left[\frac{u^2-v^2}{(\omega-v^2)^{7/2}}\right],\tag{4.26}$$

$$\mathrm{II}=\frac{-105\pi^2}{128}\frac{\rho^2}{k^7\mu^{9/2}}\int_0^1du\int_{-u}^{u}dv\left[\frac{(u^2-v^2)(1-u)}{(\omega-v^2)^{9/2}}\right],\tag{4.27}$$

$$\mathrm{III}=-\frac{105\pi^2}{64}\frac{\rho}{k^7\mu^{9/2}}(1-\mu)\int_0^1du\int_{-u}^{u}dv\left[\frac{(u^2-v^2)(1-u)u}{(\omega-v^2)^{9/2}}\right],\tag{4.28}$$

$$\mathrm{IV}=+\frac{3\pi^2}{64}\frac{1}{(k+i)^2}\frac{1}{(k^2\mu)^{5/2}}(1-2\mu)\int_0^1du\int_{-u}^{u}dv(u^2-v^2)\left[\frac{1}{(\omega-v^2)^{5/2}}-\frac{1}{(\gamma-v^2)^{5/2}}\right]$$
$$+\frac{15\pi^2}{128}\frac{1-2\mu}{(k^2\mu)^{7/2}}\int_0^1du\int_{-u}^{u}dv\left[\frac{(u^2-v^2)(1-u)}{(\omega-v^2)^{7/2}}\right]+\frac{15\pi^2}{64}\frac{1}{\rho^2}\frac{1}{(k^2\mu)^{7/2}}\int_0^1du\int_{-u}^{u}dv(u^2-v^2)[u^2(1-\mu)^2-\mu^2v^2]$$
$$\times\left[\frac{1}{(\omega-v^2)^{7/2}}-\frac{1}{(\gamma-v^2)^{7/2}}\right]+\frac{105\pi^2}{128}\frac{1}{k^7}\frac{1}{\mu^{9/2}}\int_0^1du\int_{-u}^{u}dv\left[\frac{(u^2-v^2)[u^2(1-\mu)^2-\mu^2v^2](1-u)}{(\omega-v^2)^{9/2}}\right].\tag{4.29}$$

In Eqs. (4.26)–(4.29) the following symbols have been used:

$$\mu=(1-\cos\theta)/2=\sin^2(\theta/2),$$
where θ is the angle between $\mathbf{k}_0$ and $\mathbf{k}_n$;
$$\rho=1+i/k;$$
$$\omega=u^2-(1/\mu)(u-\rho)^2;$$
$$\gamma=(u/\mu)[u(\mu-1)+(1+1/k^2)].\tag{4.30}$$

The integrals (4.26)–(4.29), while elementary, are extremely laborious to compute. We shall restrict ourselves in what follows to computing the terms corresponding to the highest power of k in the result. Superficially, one might draw the conclusion that g_{0s} behaves like $1/k^7$ as $k\rightarrow\infty$, since the only dependence of k in the integrands arises from terms which go to zero as $k\rightarrow\infty$. However, more careful examination shows that the integrals have a singularity at $u=1$ when $k\rightarrow\infty$ and thus depend strongly on k.

The terms containing the highest powers of k in Eqs. (4.26)–(4.29) are those which have the highest powers of $(\omega-u^2)$ in the denominator. Accordingly, we will examine the k-dependence of Eqs. (4.21), (4.27), and the last line of (4.29). When we do this the validity of the above statement will become obvious.

First we carry out the v integrations and retain

terms only to $1/(\omega-u^2)^{5/2}$; we get

$$\mathrm{II}=-\frac{105\pi^2}{128}\frac{\rho^2}{k^7}\frac{1}{\mu^{9/2}}\int_0^1 duu^2(1-u)\left\{\frac{2}{7}\frac{u}{\omega(\omega-u^2)^{7/2}}+\frac{12}{35}\frac{u}{\omega^2(\omega-u^2)^{5/2}}+\cdots\right\}$$
$$-u(1-u)\left\{\frac{2}{7}\frac{1}{(\omega-u^2)^{7/2}}+\frac{2}{35}\frac{1}{\omega(\omega-u^2)^{5/2}}+\cdots\right\}$$
$$=-\frac{105\pi^2}{128}\frac{\rho^2}{k^7}\frac{1}{\mu^{9/2}}\left[\int_0^1\frac{4}{35}\frac{(u^3-u^4)du}{\omega^2(\omega-u^2)^{5/2}}+\text{terms } O((\omega-u^2)^{-3/2})\right]. \tag{4.31}$$

Similarly,

$$\mathrm{III}=-\frac{105\pi^2}{64}\frac{\rho}{k^7}\frac{1}{\mu^{9/2}}(1-\mu)\left[\int_0^1\frac{4}{35}\frac{(u^4-u^5)du}{\omega^2(\omega-u^2)^{5/2}}+\text{terms } O((\omega-u^2)^{-3/2})\right] \tag{4.32}$$

and

$$\mathrm{IV}=-\frac{105\pi^2}{128}\frac{1}{k^7}\frac{1}{\mu^{9/2}}(1-\mu)^2\left[\int_0^1\frac{4}{35}\frac{(u^5-u^6)du}{\omega^2(\omega-u^2)^{5/2}}+\int_0^1\frac{u-u^2}{(\omega-u^2)^{5/2}}du+\text{terms } O((\omega-u^2)^{-3/2})\right]. \tag{4.33}$$

If one now substitutes the value of ω from Eq. (4.30) into Eqs. (4.31)–(4.32) one obtains integrals of the form

$$\int_0^1\frac{du(u^n-u^{n+1})}{(u-u_1)^2(u-u_2)^2(u-\rho)^5}, \tag{4.34}$$

where

$$u_1=\frac{\rho}{1-\mu}(1-\sqrt{\mu}),\quad u_2=\frac{\rho}{1-\mu}(1+\sqrt{\mu}).$$

If $k^2\mu\gg1$, then the highest power of k arising from terms of the form (4.34) comes from the upper limit when $(u-\rho)^{-n}$ is integrated after Eq. (4.34) is decomposed into partial fractions. In this case, the k-dependence of the other factors can be neglected. However, if $k^2\mu\lesssim1$, then there will be a strong k-dependence arising from terms of the form $(u-u_1)^{-m}$ or $(u-u_2)^{-m}$. Instead of investigating this explicitly, we will determine the k-dependence of g_0 in this range by evaluating Eqs. (4.26)–(4.29) for $\mu=0$.

After decomposing Eqs. (4.31) to (4.33) into partial fractions, we consider only terms of the form $(u-\rho)^{-5}$ and $(u-\rho)^{-4}$. If these are integrated we get

$$\mathrm{II}+\mathrm{III}+\mathrm{IV}_4=\frac{\pi^2}{128}\frac{1}{k^4}\frac{1}{\mu^2}[3-\mu^2],\quad k^2\mu\gg1. \tag{4.35}$$

To find the highest power of k when $\mu=0$, it is most convenient to return to Eqs. (4.26)–(4.29) and to set $\mu=0$ there. Again we find that II, III, IV_4 contribute to the highest power of k; the result is

$$\mathrm{II}+\mathrm{III}+\mathrm{IV}_4=5\pi^2/128;\quad \mu=0. \tag{4.36}$$

Inserting Eqs. (4.20) and (4.21) into the expression for g_{0s}, we have

$$g_{0s}=\frac{1}{k^4}\left[\frac{3}{\mu^2}-1\right],\quad k^2\mu\gg1; \tag{4.37}$$

and

$$g_{0s}=-5,\quad \mu=0. \tag{4.38}$$

Corinaldesi and Trainor[6] have computed the elastic exchange scattered cross section, with $2(1/r_1-1/r_{12})$ as the perturbation using Eq. (2.4). Their result, to first approximation, is

$$g_{0s}=\frac{16}{(1+k^2)^3}-\frac{1}{(1+k^2)^3}\left[\frac{k^4}{(1+k^2\mu)^2}+2k^2\left[\frac{\tan^{-1}(k^2\mu)^{1/2}}{(k^2\mu)^{3/2}}-\frac{1}{[k^2\mu(1+k^2\mu)]^2}\right]-\frac{3+2k^2\mu}{(1+k^2\mu)^2}+\frac{2}{(k^2\mu)^{1/2}}\tan^{-1}(k^2\mu)^{1/2}\right]. \tag{4.39}$$

In order to compare this with our result [Eqs. (4.37) and (4.38)], we select the highest power of k from Eq. (4.39), and this gives

$$g_{0a}\cong\frac{1}{k^6}\left(16-\frac{1}{\mu^2}\right),\quad k^2\mu\gg1; \tag{4.40}$$

and

$$g_{0a}=-1/k^2,\quad \mu=0. \tag{4.41}$$

5. DISCUSSION

If we were to compare the symmetric and the asymmetric perturbation procedures, we would expect that the former would give results closer to the exact solution than those obtained by the asymmetric method. There are two reasons for this. First, the symmetric perturbation method includes more of the interaction in the unperturbed Hamiltonian. Second, the formula given for the exchange scattered amplitude, using the asymmetric perturbation procedure, gives a result different from zero even when the interaction between the two electrons vanishes, whereas the symmetric perturbation does give a zero result under these circumstances. This would indicate that the first-order approximation is much poorer in the asymmetric method in the symmetric one.

The results for the two different approximations can be compared by considering Eqs. (4.37), (4.38), (4.40), (4.41), and (3.16). The meaning of these equations can be stated as follows: The direct-scattered amplitude is the same to the highest power of the energy when one uses either perturbation scheme. The fact that more of the interaction is included in the unperturbed Hamiltonian results in some additional terms, but they vanish as $k\rightarrow\infty$. The results for exchange scattering, however, exhibit quite different energy dependences in the limit of infinite k in the two different procedures. Since, as has been indicated above, the results using the asymmetric perturbation procedure are obviously incorrect, we feel that the results for exchange scattering that we have obtained must be more accurate.

In three-body scattering problems such as the scattering of neutrons by deuterons, where the masses of all three bodies are comparable, one cannot employ the symmetric perturbation procedure, and whatever calculations have been made in the Born approximation have used the asymmetric scheme. If the conclusions arrived at here could be extrapolated to these problems, there must be some doubt as to the validity of the results already obtained for those cases where exchange scattering plays a significant role. For such problems, other approximation methods should be investigated.

The direct-scattered amplitude in the case of elastic scattering by hydrogen atoms is so much larger than the exchange-scattered amplitude, that there is no possibility of verifying experimentally the theoretical difference between the results of the symmetric and the asymmetric methods.

There is a possibility, however, of checking experimentally the effectiveness of the type of perturbation method presented here. Corinaldesi and Trainor[6] have shown that some inelastic scattering processes have approximately the same energy dependence for the direct- and exchange-scattered amplitude. If the symmetric perturbation theory will alter substantially the exchange-scattered term for this process, then an experiment measuring the cross section for this process will enable us to choose between the two formulations. This investigation is being undertaken.

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APPENDIX

We carry out here the detailed evaluation of the integral (4.24) because it exhibits not only the method of Feynman,[11] but also illustrates how we handle the additional complication of differentiating with respect to k_0 and k_n. We repeat Eq. (4.24) here:

$$\frac{\mathrm{III}}{k+i}=-\frac{1}{2}\frac{\partial}{\partial k_0}4!\int\frac{x_1x_3\delta(x_1+x_2+x_3-1)dx_1dx_2dx_3d\mathbf{K}}{\{[K^2-(k+i)^2]x_1+[1+K^2+k^2-2(\mathbf{K},\mathbf{k}_0)]x_2+[1+|\mathbf{K}-\mathbf{k}_n|^2]x_3\}^5}$$
$$-\frac{1}{2}\frac{\partial}{\partial k_n}4!\int\frac{x_1x_2\delta(x_1+x_2+x_3-1)dx_1dx_2dx_3d\mathbf{K}}{\{[K^2-(k+i)^2]x_1+(1+|\mathbf{K}-\mathbf{k}_0|^2)x_2+[1+K^2-2(\mathbf{K},\mathbf{k}_n)+k^2]x_3\}^5}. \tag{A.1}$$

Now we let $\mathbf{P}=\mathbf{K}-\mathbf{k}_0x_2-\mathbf{k}_nx_3$ and carry out the integration with respect to x_1. Then we differentiate with respect to k_0 and k_n to obtain

$$\frac{\mathrm{III}}{(k+i)}=-5!k\int\frac{(1-(x_2+x_3))x_2x_3(x_2+x_3)(1+\xi)dx_2dx_3d\mathbf{P}}{(P^2+\Theta^2)^6} \tag{A.2}$$

where $\xi=\cos\theta$

$$\Theta^2=4k^2x_2x_3\mu-[k(x_2+x_3)-(k+i)]^2.$$

We now can carry out the integrations with respect to $\mathbf{P}$ immediately, to obtain

$$\mathrm{III}=-\frac{105\pi^2}{8}k(k+i)(1-\mu)\int_0^1dx_2\int_0^{1-x_2}dx_3\frac{(x_2+x_3)(1-(x_2+x_3))x_2x_3}{[4k^2x_2x_3\mu-(k(x_2+x_3)-(k+i))^2]^{9/2}}. \tag{A.3}$$

Now let $x_2+x_3=u$, $x_2-x_3=v$. Then

$$\mathrm{III}=-\frac{105\pi^2}{64}\frac{\rho}{k^7\mu^{9/2}}(1-\mu)\int_0^1du\int_{-u}^{u}dv\frac{(u^2-v^2)(1-u)u}{(\omega-v^2)^{9/2}}. \tag{A.4}$$

This is the result given in the text.