

e^- -H scattering for a wider range of energy

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An integral form of the close-coupling approximation has been applied to the scattering of electrons by hydrogen atoms with the retention of only the 1s state, the effect of exchange being included. Results for the differential and the total cross sections have been obtained from 1 to 500 eV. The calculated results have been compared with the experimental findings and other theoretical results and are found to be fairly reliable throughout the entire energy range. The present results differ from Born values by about 4% even at 500 eV.

INTRODUCTION

In the study of electron-atom collision problems, the maximum number of theoretical investigations have been centered around the e^- -H scattering process because of its simplicity and the availability of exact wave functions. Recent experimental measurements of Teubner *et al.*¹ of the differential cross sections of the e^- -H system at low and moderately high incident energies have given further impetus to the theoretical works. For low incident energies there are some methods² which yield satisfactory results. Some methods³ have also been employed to investigate the electron-hydrogen system in the intermediate- and high-incident-energy regions with promising results. However, none of these methods furnishes uniformly satisfactory results for all incident energies.

Here we are interested in finding a method that may be applicable to a wider range of energies. Several theoretical investigations⁴ have been carried out to study the e^- -H system by using the close-coupling approximation.⁵ The close-coupling method is based on the expansion of the total wave function into an infinite number of eigenstates of the target atom. In practice, it is not possible to include more than a limited number of bound states. In actual calculations, one has to solve a set of coupled integrodifferential equations for each value of the total angular momentum. The number of coupled equations depends on the number of bound states taken. At the time of calculations special devices have to be developed to incorporate the boundary conditions and to evaluate the integrals by the iterative method. Naturally, computational labor is enormous. The condition becomes worse when the incident energy increases, since the effects of the higher partial waves become important with the increase of the incident energy. It is not too practicable to go beyond⁴ moderate incident energies on account

of this fact. The convergence of the iterative method is of prime importance. Near the excitation threshold, Burke *et al.*⁴ have encountered convergence difficulties. The close-coupling method, which is considered to be theoretically sound, may be suitable for a wider range of energies if one gets rid of these difficulties.

In view of the situation, an integral form of the close-coupling method as used by Ghosh and Basu⁶ for the investigation of e^- -H scattering is a suitable alternative. This method incorporates the boundary conditions automatically and the result can be obtained quite straightforwardly, whereas in the differential approach one has to be careful at every point of the radial variable. Further, this formalism has been found to be free from any convergence difficulty throughout the entire range of energies. Moreover, the computer time required for this method will be less than the conventional close-coupling method. Under these circumstances the present method of solution, we think, is less laborious than the conventional close-coupling method and is applicable to a wider range of energies. For the sake of simplicity, however, Ghosh and Basu⁶ neglected the rearrangement channels as well as the excitations of the target atom. Here, we have applied this formalism to investigate the e^- -H scattering problem including the effect of exchange which is considered to be vital at low and intermediate energies.

THEORY

We present here a brief derivation of the integral form^{6,7} of the close-coupling equations. We choose particles 1 and 2 to be the electrons and the particle 3 the proton so that (in atomic units)

$$V_{13} = -\frac{1}{r_1}, \quad V_{23} = -\frac{1}{r_2}, \quad V_{12} = \frac{1}{|r_1 - r_2|}.$$

The close-coupling equations may be written as^{4,7}

$$(E - e_{n'} - T_1)F_{n'}^{\pm} = \sum_{n=1}^N \hat{V}_{n'n} F_n^{\pm}, \quad (1)$$

where N is the number of bound states taken, E is the total energy of the system, $e_{n'}$ is the energy of the hydrogen bound state $\phi_{n'}$, and T_1 is the kinetic-energy operator for incident electron 1. $\hat{V}_{nn'}$ may be expressed as

$$\hat{V}_{nn'} = \hat{A}_{n'n}^d + \hat{A}_{n'n}^{en}(E), \quad (2)$$

where

$$\hat{A}_{n'n}^d = \int \phi_n^*(\vec{r}_2)(V_{13} + V_{12})\phi_n(\vec{r}_2) d\vec{r}_2 \quad (3)$$

and $\hat{A}_{n'n}^{en}$ is the exchange potential operator given by

$$A_{n'n}^{en}F(\vec{r}_1) = \int \phi_n^*(\vec{r}_2)(H - E)F(\vec{r}_2) d\vec{r}_2 \phi_n(\vec{r}_1), \quad (4)$$

H being the total Hamiltonian of the system. We introduce the set of solutions $F_n^{(n)}$ ($n=1, 2, \dots, N$) which corresponds asymptotically to a plane wave with momentum incident in the bound state ϕ_n , together with outgoing spherical waves in all open channels. The Lipmann-Schwinger equations

$$\langle \vec{k}'n' | Y^{\pm} | \vec{k}n \rangle = \langle \vec{k}'n' | B^{\pm} | \vec{k}n \rangle + \sum_{n''} \int d\vec{k}'' \frac{\langle \vec{k}'n' | B^{\pm} | \vec{k}''n'' \rangle \langle \vec{k}''n'' | Y^{\pm} | \vec{k}n \rangle}{E + i\epsilon - E''}. \quad (8)$$

In this paper we have neglected the coupling to the excited states of the target and as a result, the summation over n'' has been omitted from Eq. (8). The matrix element of B^{\pm} may be expressed as

$$\langle \vec{k}' 1s | B^{\pm} | \vec{k} 1s \rangle = -(1/4\pi^2) f^{B\pm}(\vec{k}', \vec{k}), \quad (9)$$

where $f^{B\pm} = f^{B\pm} g^0$; f^B is the familiar Born amplitude, and on the energy shell g^0 is the Oppenheimer exchange amplitude. In a similar way, we denote the matrix elements of Y^{\pm} as

$$\langle \vec{k}' 1s | Y^{\pm} | \vec{k} 1s \rangle = -(1/4\pi^2) f^{\pm}(\vec{k}', \vec{k}), \quad (10)$$

so that f^+ and f^- are the required normalized singlet and triplet scattering amplitudes. With the help of Eqs. (9) and (10), we can write Eq. (8) as

$$f^{\pm}(\vec{k}', \vec{k}) = f^{B\pm}(\vec{k}', \vec{k}) - \frac{1}{4\pi^2} \times \int d\vec{k}'' \frac{f^{B\pm}(\vec{k}', \vec{k}'') f^{\pm}(\vec{k}'', \vec{k})}{E + i\epsilon - E''}. \quad (11)$$

Now the pole term in Eq. (11) has a δ -function part and a principal-value part:

satisfied by them are

$$\begin{aligned} F_{n'}^{(n)\pm} &= \delta_{n'n} |\vec{k}\rangle + \sum_{m=1}^N \frac{1}{E + i\epsilon - e_{n'} - T_1} \hat{V}_{n'm} F_m^{(n)\pm} \\ &= \delta_{n'n} |\vec{k}\rangle + \sum_{m=1}^N \int d\vec{k}' |\vec{k}'\rangle \frac{1}{E + i\epsilon - E'} \\ &\quad \times \langle \vec{k}' | V_{n'm} | F_m^{(n)\pm} \rangle. \end{aligned} \quad (5)$$

We denote the amplitude for transition from state n to state n' by $\langle \vec{k}'n' | Y^{\pm} | \vec{k}n \rangle$ with \vec{k}' the final momentum. From a comparison with the asymptotic form of Eq. (5), the transition amplitudes can be written as

$$\langle \vec{k}'n' | Y^{\pm} | \vec{k}n \rangle = \sum_{m=1}^N \langle \vec{k}' | \hat{V}_{n'm}^{\pm} | F_m^{(n)\pm} \rangle. \quad (6)$$

We now introduce the operators B whose matrix elements are given by

$$\langle \vec{k}'n' | B^{\pm} | \vec{k}n \rangle = \langle \vec{k}' | V_{n'n}^{\pm} | \vec{k} \rangle. \quad (7)$$

On using relations (6) and (7) one can obtain the required integral form of the close-coupling equations as

$$\frac{1}{E + i\epsilon - E''} = -i\pi\delta(E - E'') + \frac{P}{E - E''}. \quad (12)$$

With the help of Eq. (12), Eq. (11) may be written as

$$\begin{aligned} f^{\pm}(\vec{k}', \vec{k}) &= f^{B\pm}(\vec{k}', \vec{k}) + \frac{i}{4\pi} \int d\vec{k}'' f^{B\pm}(\vec{k}', \vec{k}'') \delta(E - E'') \\ &\quad \times f^{\pm}(\vec{k}'', \vec{k}) - \frac{P}{4\pi^2} \int d\vec{k}'' \frac{f^{B\pm}(\vec{k}', \vec{k}'') f^{\pm}(\vec{k}'', \vec{k})}{E - E''} \end{aligned} \quad (13)$$

After the partial-wave analysis, these three-dimensional integral equations are converted into one-dimensional integral equations and the resulting form is given by

$$\begin{aligned} f_i^{\pm}(k', k) &= f_i^{B\pm}(k', k) + i f_i^{B\pm}(k', k) f_i^{\pm}(k, k) \\ &\quad + \frac{2}{\pi} P \int k'' dk'' \frac{f_i^{B\pm}(k', k'') f_i^{\pm}(k'', k)}{k''^2 - k^2}, \end{aligned} \quad (14)$$

with

$$f_i^{\pm}(k', k) = \frac{1}{k} \sum_l (2l+1) f_l^{\pm}(k', k) P_l(\hat{k}' \cdot \hat{k}),$$

and a similar expression for $f^{B\pm}(\vec{k}', \vec{k})$. It may be mentioned that on using the Faddeev equations Sloan and Moore⁷ and Sil and his co-workers⁸ obtained an approximate on-shell form which is identical to the expression given by Eq. (14), omitting the principal-value part. If one omits the principal-value part and neglects the effect of the exchange, Eq. (14) reduces to the unitarized Born approximation.

In the Appendix, we have given the partial-wave analysis of g^0 .

RESULTS

For a fixed value of k corresponding to a particular incident energy, the two uncoupled one-dimensional integral equations given by Eq. (14) have been solved for each value of the angular momentum. The Gaussian quadrature method has been used for the integration of the principal-value part. The integration range over 0 to ∞ has been divided into two parts, i.e., from 0 to $2k$ and $2k$ to ∞ , and an even number of points is used to calculate the first part. The integral equation is converted into a suitable matrix equation which is solved numerically. The on-shell value of the solution gives the physical amplitude. The convergence of the results has been tested by increasing the number of Gaussian points. The first Born and Born-Oppenheimer results have been reproduced as a check of the program.

In Fig. 1, we have given our results for the differential cross sections for the scattering of electrons by the hydrogen atom and compared them with results obtained by Burke *et al.*⁴ as well as the experimental points measured by Teubner *et al.*¹ and Gilbody *et al.*⁹ at 9.4 eV. In Fig. 2, we have plotted the present values of the differential cross sections at 12.0 eV along with the corresponding results obtained using the $1s-2s-2p$ close-coupling approximation (CCA); the experimental findings of Teubner *et al.*¹ have been given for comparison. The observed sharp rise in the

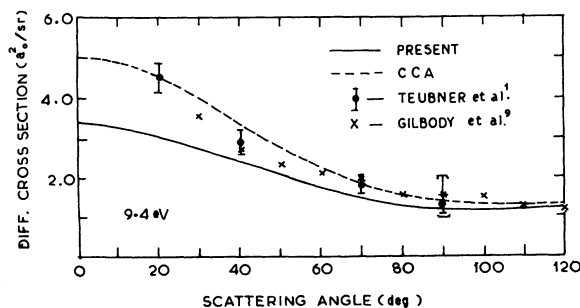


FIG. 1. Differential cross sections for e -H scattering at 9.4 eV.

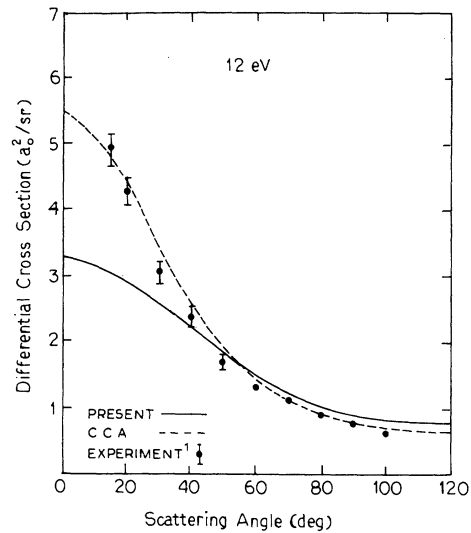


FIG. 2. Differential cross sections for e -H scattering at 12 eV.

forward direction as confirmed by the CCA calculations is not represented by our curves. This steep rise in the forward direction is presumably due to the effect of polarization.² The present formulation excludes the coupling to higher excited states and as such it cannot take proper account of the polarization effect. This effect is expected to be quite important at the energy selected for comparison in Figs. 1 and 2. Therefore the discrepancy between our results and the experimental findings,^{1,9} as well as the values obtained by

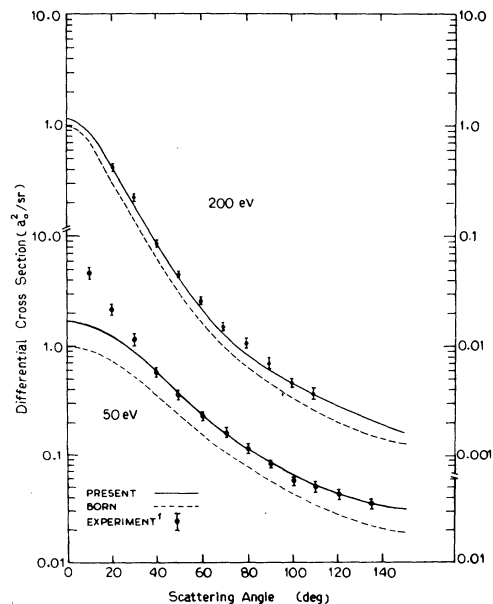


FIG. 3. Differential cross sections for e -H scattering at 50 and 200 eV.

Burke *et al.*⁴ can be explained. However, our values are approximately 3.5 times higher than those calculated from the Born approximation at the zero-degree scattering angle. From the 40° scattering angle and onward, our curves are in good agreement with the experimental findings. It may be mentioned that the results of the Born approximation are approximately five to six times smaller than those obtained by us at the backward scattering angle.

In Figs. 3 and 4, we show our curves for the differential cross sections along with the corresponding results of the Born approximation and compare them with the experimental points.¹ At 50 eV our curve shows good agreement with the experimental findings from 40° onward. It may be mentioned that the results of CCA calculated by Scott¹⁰ (not given in the figures) at 50 eV are very close to our curve throughout the entire range of the scattering angle except for a slight discrepancy in the forward direction. The agreement between our results and the experimental findings at 100 eV is satisfactory for a scattering angle of 30° and onward. At 200 eV there are no experimental points below 20° and beyond this angle our curve rather coalesces with the available experimental points. It appears that the region of discrepancy near the forward direction shrinks with increasing energy. The results obtained by the Born approximation always lie below our values as well as the experimental findings although the slopes of the Born curves are more or less the same as ours. Even at 500 eV (Fig. 5), the Born results differ in magnitude by about 4%.

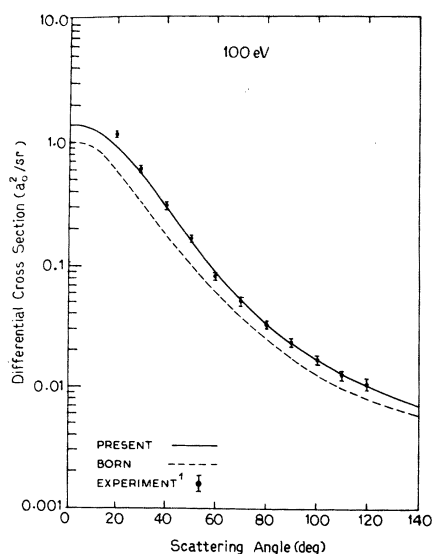


FIG. 4. Differential cross section for e -H scattering at 100 eV.

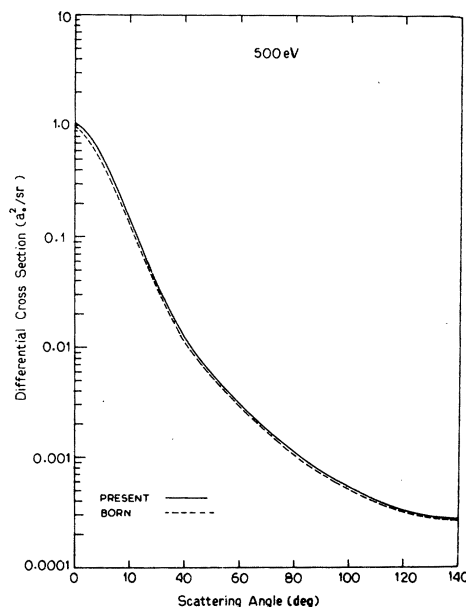


FIG. 5. Differential cross section for e -H scattering at 500 eV.

Table I contains the singlet and triplet partial scattering amplitudes f^+ and f^- up to $l=14$ (spin statistical factors are not included) at 200 and 500 eV. It is apparent from the table that the effect of exchange is not vanishingly small even at 500 eV. This feature has also been noticed by Sloan and Moore⁷ and Sil and Ghosh.⁸

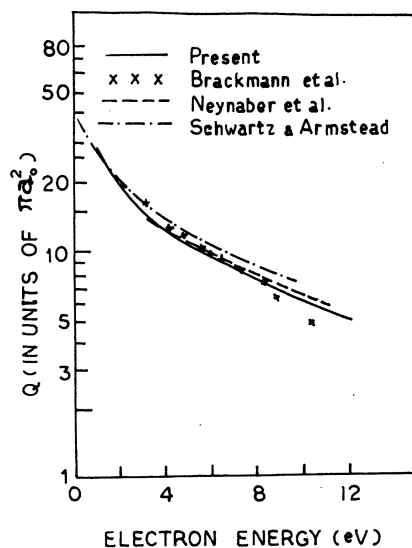


FIG. 6. Total cross section for e -H scattering. Results of Schwartz and Armstead are the combined results of s -wave calculations of Schwartz and p -wave calculations of Armstead.

TABLE I. Real and imaginary parts of partial singlet and triplet amplitudes^a (in units of a_0). Spin statistical factors are not included.

Energy l	200 eV				500 eV			
	Singlet f_e^+		Triplet f_e^-		Singlet f_e^+		Triplet f_e^-	
	Re	Im	Re	Im	Re	Im	Re	Im
0	3.440(-1)	1.372(-1)	3.550(-1)	1.479(-1)	4.073(-1)	2.100(-1)	4.362(-1)	2.556(-1)
1	2.096(-1)	4.603(-2)	2.226(-1)	5.228(-2)	2.153(-1)	4.815(-2)	2.583(-1)	7.187(-2)
2	1.390(-1)	1.970(-2)	1.506(-1)	2.322(-2)	1.190(-1)	1.436(-2)	1.525(-1)	2.938(-2)
3	9.567(-2)	9.237(-3)	1.052(-1)	1.119(-2)	6.813(-2)	4.664(-3)	9.106(-2)	8.356(-3)
4	6.716(-2)	4.531(-3)	7.470(-2)	5.610(-3)	3.987(-2)	1.592(-3)	5.482(-2)	3.015(-3)
5	4.770(-2)	2.281(-3)	5.345(-2)	2.876(-3)	2.365(-2)	5.594(-4)	3.321(-2)	1.104(-3)
6	3.415(-2)	1.167(-3)	3.862(-2)	1.494(-3)	1.415(-2)	1.999(-4)	2.019(-2)	4.078(-4)
7	2.458(-2)	6.044(-4)	2.797(-2)	7.829(-4)	8.498(-3)	7.222(-5)	1.230(-2)	1.513(-4)
8	1.775(-2)	3.151(-4)	2.031(-2)	4.126(-4)	5.125(-3)	2.626(-5)	7.502(-2)	5.628(-5)
9	1.285(-2)	1.652(-4)	1.477(-2)	2.183(-4)	3.097(-3)	9.592(-6)	4.578(-3)	2.096(-5)
10	9.322(-3)	8.691(-5)	1.076(-2)	1.158(-4)	1.874(-3)	3.512(-6)	2.794(-3)	7.804(-6)
11	6.771(-3)	4.585(-5)	7.845(-3)	6.154(-5)	1.135(-3)	1.288(-6)	1.704(-3)	2.905(-6)
12	4.922(-3)	2.423(-5)	5.722(-3)	3.274(-5)	6.877(-4)	4.729(-7)	1.039(-3)	1.080(-6)
13	3.581(-3)	1.282(-5)	4.174(-3)	1.743(-5)	4.167(-4)	1.737(-7)	6.335(-4)	4.013(-7)
14	2.606(-3)	6.792(-6)	3.047(-3)	9.281(-6)	2.525(-4)	6.378(-8)	3.859(-4)	1.489(-7)

^a Number in parentheses in each entry is the power of ten by which the amplitude value should be multiplied.

Figure 6 represents our total cross section from 1 to 12 eV along with the theoretical results of Schwartz² and Armstead.¹¹ The experimental findings of Neynaber *et al.*¹² and Brackmann and Fite¹³ have also been included in Fig. 6. Our curves are the same as obtained by John⁴ using conventional CCA-retaining 1s states only. The present value of the total cross section at 1 eV is $27.518\pi a_0^2$. This value, as expected, is slightly greater than the Schwartz value and also greater than the value obtained by Temkin and Lamkin² and the 1s-2s-2p CCA⁴ (not given in Fig. 1). The present values of the total cross section in the energy range 10–500 eV are given in Fig. 7 along with the values of Born approximation and the results of Burke *et al.*⁴ using the 1s-2s-2p CCA. From Figs. 6 and 7, we can see that near the excitation threshold, our values deviate most from the more accurate theoretical results and the experimental findings. As we move away from this energy region, the difference steadily decreases. This feature has also been noticed for differential cross sections. The difference between the Born curve and our curve steadily decreases with increasing energy. Even at 500 eV, our values for the total cross section differ from the Born result by about 4%. Similar discrepancy has also been reported by Banerjee *et al.*⁸ for the positron-hydrogen scattering and by Byron and Joachain¹⁴ for electron-hydrogen collisions.

CONCLUSION

Throughout the entire energy range, from 1 to 500 eV, the present formalism furnishes fairly

reliable results. This method of calculation enables one to apply the close-coupling approximation to intermediate- and high-energy regions. There is a general belief that the Born approximation is valid for $E > 200$ eV for the electron-hydrogen scattering problem. The present results,

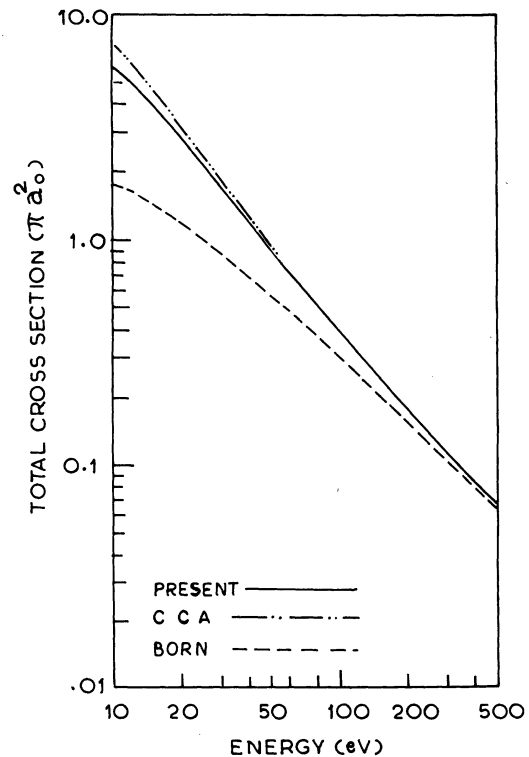


FIG. 7. Total cross section for e -H scattering.

both for the total and the differential cross sections, differ from the Born results by about 4% at energies as high as 500 eV. This casts doubt as to the energy region where the first Born ap-

proximation is expected to be accurate. Further calculations including a larger number of states are necessary to settle the high-energy behavior of the cross sections.

APPENDIX

Our aim is to reduce the exchange partial-wave amplitude g_l^0 to a suitable form for numerical calculations; the analysis for the Born amplitude f^B is straightforward. The expression for the exchange amplitude g^0 is of the form

$$g^0 = (1/2\pi) \int \int e^{-\beta r_2} e^{-i\vec{q}\cdot\vec{r}_1} (H-E) e^{-\alpha r_1} e^{i\vec{p}\cdot\vec{r}_2} d\vec{r}_2 d\vec{r}_1 \\ = - (1/2\pi) \int \int e^{-\beta r_2} e^{-i\vec{q}\cdot\vec{r}_1} [(1/r_{12}) - (1/r_2) + (E'-E)] e^{-\alpha r_1} e^{i\vec{p}\cdot\vec{r}_2} d\vec{r}_2 d\vec{r}_1 .$$

On the energy shell, the final-state energy E' is equal to E and g^0 is then the well-known Oppenheimer amplitude. The partial-wave amplitude is given by

$$g_l^0 = \frac{1}{2} p \int_{-1}^{+1} g_l^0 P_l(t) dt ,$$

where

$$t = \hat{p} \cdot \hat{q} .$$

The partial-wave analysis for the parts of the amplitude containing $1/r_2$ and $(E'-E)$ can be easily performed, and we give the reduction only for the part containing $1/r_{12}$. This part, denoted by A , may be expressed as¹⁵

$$A = 8 \frac{\partial}{\partial \alpha} \frac{\partial}{\partial \beta} \int \frac{d\vec{k}}{k^2 [(k-p)^2 + \beta^2] [(k-q)^2 + \alpha^2]} ;$$

using the parametrization technique, A can be written as

$$A = 4 \frac{\partial}{\partial \alpha} \frac{\partial}{\partial \beta} \int_{-1}^{+1} dz \int \frac{d\vec{k}}{k^2 [(\vec{k}-\vec{p})^2 + \lambda^2]^2} ,$$

where

$$\vec{p} = \frac{1}{2} \vec{p}(1-z) - \frac{1}{2} \vec{q}(1+z) ,$$

$$\lambda^2 = M + Nt ,$$

with

$$M = \frac{1}{4} (p^2 + q^2) (1-z^2) + \frac{1}{2} (\alpha^2 + \beta^2) z + \frac{1}{2} (\alpha^2 + \beta^2) ,$$

$$N = \frac{1}{2} p q (1-z^2) .$$

Performing the integration¹⁶ with respect to \vec{k} , we have

$$A = 4\pi^2 \frac{\partial}{\partial \alpha} \frac{\partial}{\partial \beta} \int_{-1}^{+1} \frac{dz}{(M+Nt)^{1/2} (D+Ez)} ,$$

where

$$D = p^2 + q^2 + \alpha^2 + \beta^2 ,$$

$$E = q^2 + \alpha^2 - p^2 - \beta^2 .$$

Multiplying both sides by $P_l(t)$ and integrating with respect to dt , we have

$$\int_{-1}^{+1} A P_l(t) dt = 4\pi^2 \frac{\partial}{\partial \alpha} \frac{\partial}{\partial \beta} \frac{2}{2l+1} \int_{-1}^{+1} \frac{h^l}{c(D+Ez)} dz ,$$

where

$$h = (1/2c) [(M+N)^{1/2} - (M-N)^{1/2}] ,$$

with

$$c = \frac{1}{2} [(M+N)^{1/2} + (M-N)^{1/2}] .$$

It should be noted that there is an error in the partial-wave analysis of the scattering amplitude given by Sil and Ghosh.⁸

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