Variational Calculation of Electron Scattering by a Static Potential*†

LYMAN MOWER‡
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts
(Received March 24, 1955)

The Schwinger variational method, for the approximate determination of scattering amplitude, is tested for accuracy in the case of the elastic scattering of electrons from the static potential $V(\mathbf{r}) = -e^2V_0e^{-\lambda r}/r$, by using eight different forms of trial wave functions. The results are compared by checking the closeness of fit of the associated scattering amplitude with an exact solution to the problem. In the course of the calculation a number of expressions, of use in more complicated problems, were obtained and are here recorded. The parameter values used in the test were $a_0\lambda = 8/3$, $k^2 = (0.72\lambda)^2$, $V_0 = 7.8$, where a_0 is the first Bohr orbit radius for hydrogen.

1. INTRODUCTION

IN the application of variational methods to scattering problems the algebraic and numerical computations have been directed mainly toward the determination of either the first few phase shifts or the total scattering cross section.[1] However, for a given trial function the determination of the scattering amplitude imposes a stricter test on the reliability of the trial wave function than does the determination of the first few phase shifts or the total scattering amplitude.

We apply here the Schwinger variational method for the approximate determination of the scattering amplitude for the elastic scattering of electrons from a static potential.[2] Several different trial wave functions are compared for possible application to similar problems; the criterion used for "best form" consists in the closeness of fit of the associated scattering amplitude with a numerical solution to the problem.

For reference we include a brief description of the Schwinger variational method as applied to scattering problems.

2. PRELIMINARY REMARKS

The scattering of an electron by a potential $V(\mathbf{r})$ is described by a solution to the integral equation[3]

$$\psi_i(\mathbf{r}) = e^{i\mathbf{k}_i\cdot\mathbf{r}} - \frac{2m}{\hbar^2}\int \frac{G(\mathbf{r},\mathbf{r}')}{4\pi} V(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}', \quad (1)$$

where

$$G(\mathbf{r},\mathbf{r}') = e^{ikR}/R, \quad R = |\mathbf{r}-\mathbf{r}'|, \quad (2)$$

is the free space Green function for the Helmholtz equation, $E = \hbar^2k^2/2m$ is the energy of the incident electron, m is its mass, and $\hbar$ is Plank's constant divided by 2π. The vector $\mathbf{k}_i = k\mathbf{n}_i$, where the unit vector $\mathbf{n}_i$ specifies the direction of incidence; the vector $\mathbf{r} = r\mathbf{n}$ is the radius vector which specifies the position of the electron. Substituting into (1) the asymptotic form of the Green function,[3]

$$G(\mathbf{r},\mathbf{r}') \to \exp(ikr - ik\mathbf{n}\cdot\mathbf{r}')/r, \quad r \gg r', \quad (3)$$

we obtain

$$\psi_i(\mathbf{r}) \to e^{i\mathbf{k}_i\cdot\mathbf{r}} + f(\mathbf{n},\mathbf{n}_i)e^{ikr}/r, \quad r \gg r', \quad (4)$$

where

$$f(\mathbf{n},\mathbf{n}_i) = -\frac{m}{2\pi\hbar^2}\int \exp(-ik\mathbf{n}\cdot\mathbf{r}')V(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}' \quad (5)$$

is the scattering amplitude and is the quantity which we wish to characterize by a variational method. The quantity $|f(\mathbf{n},\mathbf{n}_i)|^2$ represents the density of the current scattered by the potential $V(\mathbf{r})$ in the direction $\mathbf{n}$ for a stream of particles of unit current density incident in the direction $\mathbf{n}_i$.

Using the integral equation (1) and the definition of the scattering amplitude (5), we may rewrite the expression for the scattering amplitude as[4]

$$[f(\mathbf{n}_s,\mathbf{n}_i)] = -\frac{1}{4\pi}\Bigg\{\int e^{-i\mathbf{k}_s\cdot\mathbf{r}'}U(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}' + \int e^{i\mathbf{k}_i\cdot\mathbf{r}}U(\mathbf{r})\psi_{-s}(\mathbf{r})d\mathbf{r} - \int \psi_{-s}(\mathbf{r})U(\mathbf{r})\psi_i(\mathbf{r})d\mathbf{r} - \frac{1}{4\pi}\int\int \psi_{-s}(\mathbf{r})U(\mathbf{r})G(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}d\mathbf{r}'\Bigg\}, \quad (6)$$

where $U(\mathbf{r}) = 2mV(\mathbf{r})/\hbar^2$, and where the wave function

* This work was supported in part by the Office of Naval Research.
† This work is based in part on material submitted in partial fulfillment for the Ph.D. degree at Massachusetts Institute of Technology.
‡ Now at the Electronic Defense Laboratory, Box 205, Mountain View, California.
[1] L. Hulthén, Kgl. Fysiograf. Sallskap. Lund. Förh. **14**, 1 (1944); W. Kohn, Phys. Rev. **74**, 1763 (1948); S. S. Huang, Phys. Rev. **76**, 477 (1949); H. S. W. Massey and B. L. Moiseiwitsch, Proc. Roy. Soc. (London) **A205**, 483 (1951); G. A. Erskine and H. S. W. Massey, Proc. Roy. Soc. (London) **A212**, 521 (1952); S. Altschuler, Phys. Rev. **89**, 1278 (1953); H. Boyet and S. Borowitz, Phys. Rev. **93**, 1225 (1954).
[2] B. A. Lippman and J. Schwinger, Phys. Rev. **79**, 469 (1950); T. Kahan and G. Rideau, J. phys. radium **13**, 326 (1952); E. Gerjuoy and D. S. Saxon, Phys. Rev. **85**, 939 (1952) have used a form like the one listed as ϕ_{i7} in Eq. (9).
[3] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949), second edition, p. 116.
[4] See reference 2, and P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), p. 804.

$\psi_{-s}(\mathbf{r})$ represents a solution to (1) for a plane wave incident in the direction $(-\mathbf{n}_s)$, where $\mathbf{k}_s=k\mathbf{n}_s$. We note that $[f(\mathbf{n}_s,\mathbf{n}_i)]$ is an exact expression for the scattering amplitude $f(\mathbf{n}_s,\mathbf{n}_i)$.

For the approximate determination of the scattering amplitude, the procedure followed is to substitute into the functional $[f(\mathbf{n}_s,\mathbf{n}_i)]$ a set of functions ϕ which satisfy or nearly satisfy the integral equation (1). These functions are termed trial functions. Then those trial functions which differ from the exact value of ψ to the first order in $\delta\psi$ yield values of the functional $[f(\mathbf{n}_s,\mathbf{n}_i)]$ which differ from the exact value of $[f(\mathbf{n}_s,\mathbf{n}_i)]$, i.e., the scattering amplitude, by terms proportional to $(\delta\psi)^2$. Hence, the difference between the scattering amplitude and the above value of the functional is small to the second order in $(\delta\psi)$.

By introducing trial functions of the form

$$\phi(\mathbf{r})=\sum_{n=0}^{N} C_n\chi_n(\mathbf{r}) \tag{7}$$

into (6), where the C_n are unknown constants and the $\chi_n(\mathbf{r})$ are known functions of $\mathbf{r}$, the functional $[f(\mathbf{n}_s,\mathbf{n}_i)]$ becomes a function of the C_n. Thus the necessary condition that $[f(\mathbf{n}_s,\mathbf{n}_i)]$ be stationary with respect to small variations of $\phi_i(\mathbf{r})$ and $\phi_{-s}(\mathbf{r})$ about $\psi_i(\mathbf{r})$ and $\psi_{-s}(\mathbf{r})$ is that

$$\partial[f(\mathbf{n}_s,\mathbf{n}_i)]/\partial C_n=0,\quad n=0,1,\cdots N. \tag{8}$$

The foregoing equations consist of a set of $N+1$ simultaneous, linear equations sufficient to determine uniquely the set of $N+1$ unknowns. By assuming a trial function of the form (7), the resultant expression for the scattering amplitude $[f(\mathbf{n}_s,\mathbf{n}_i)]$ is independent of the normalization of the trial wave function $\phi(\mathbf{r})$.

Clearly the method is only as good as the choice of the trial function. If we know the exact function, then we obtain the extremum value of $[f(\mathbf{n}_s,\mathbf{n}_i)]$, i.e., the scattering amplitude, exactly. However, if we make a bad choice in the trial function, then the error in the functional will be correspondingly augmented.

We note that inasmuch as the Green function (2) is not definite, the extremum point of the function $[f(\mathbf{n}_s,\mathbf{n}_i)]$ may be either a maximum, a minimum, or a saddle point.[5]

3. APPLICATION OF THE VARIATIONAL METHOD

For the trial wave functions

$$\begin{aligned}
&\phi_{i1}(\mathbf{r})=C_0e^{i\mathbf{k}_i\cdot\mathbf{r}},\\
&\phi_{i2}(\mathbf{r})=C_0e^{i\mathbf{k}_i\cdot\mathbf{r}}+C_1e^{i\mathbf{k}_i\cdot\mathbf{r}-\lambda r},\\
&\phi_{i3}(\mathbf{r})=C_0e^{i\mathbf{k}_i\cdot\mathbf{r}}+C_1e^{-\lambda r},\\
&\phi_{i4'}(\mathbf{r})=C_0e^{i\mathbf{k}_i\cdot\mathbf{r}}+C_1e^{-\lambda r}+iC_2r\lambda e^{-\lambda r/2}(\mathbf{n}_i\cdot\mathbf{n}),\\
&\phi_{i5}(\mathbf{r})=C_0e^{i\mathbf{k}_i\cdot\mathbf{r}}+C_1j_0(kr),\\
&\phi_{i6}(\mathbf{r})=C_0e^{i\mathbf{k}_i\cdot\mathbf{r}}+C_1j_0(kr)+iC_2j_1(kr)(\mathbf{n}_i\cdot\mathbf{n}),\\
&\phi_{i7}(\mathbf{r})=C_0e^{i\mathbf{k}_i\cdot\mathbf{r}}+C_1e^{-i\mathbf{k}_i\cdot\mathbf{r}},\\
&\phi_{i8}(\mathbf{r})=C_0e^{i\mathbf{k}_i\cdot\mathbf{r}}+C_1e^{-i\mathbf{k}_i\cdot\mathbf{r}}+C_2j_0(kr),\\
&\phi_{i9'}(\mathbf{r})=\phi_{i8}(\mathbf{r})\ [\text{see paragraph below Eq. (18)}],
\end{aligned} \tag{9}$$

where $j_n(x)$ is the nth order spherical Bessel function, and for the potential

$$V(\mathbf{r})=-e^2V_0e^{-\lambda r}/r, \tag{10}$$

approximate expressions for the scattering amplitude were calculated using the stationary form (6). We note that the trial wave functions $\phi_{-s}(\mathbf{r})$ are obtained from the $\phi_i(\mathbf{r})$ by replacing the vector $\mathbf{k}_i$ by $(-\mathbf{k}_s)$; for simplification, we have introduced the notation

$$\begin{aligned}
&[f(\theta)]=[f(\mathbf{n}_s,\mathbf{n}_i)],\\
&\theta=\arccos(\mathbf{n}_i\cdot\mathbf{n}_s),\\
&x=2k/\lambda,\\
&c=\sin(\theta/2).
\end{aligned} \tag{11}$$

As an illustration of the procedure we calculate $[f(\theta)]$ for the trial wave function ϕ_7 [see (9)]; thus, upon performing the indicated integrations, we obtain

$$\begin{aligned}
[f_7(\theta)]=f_B(\theta)\{2C_0+2C_1\alpha-(C_0^2+C_1^2)[1-T_0(\theta)]\\
-2C_0C_1\alpha[1-T_0(\pi-\theta)]\},
\end{aligned} \tag{12}$$

where[3]

$$f_B(\theta)=-\frac{1}{4\pi}\int e^{i(\mathbf{k}_i-\mathbf{k}_s)\cdot\mathbf{r}}U(\mathbf{r})d\mathbf{r}=(U_0/\lambda)(x^2c^2+1)^{-1} \tag{13}$$

is the first Born approximation for the potential considered, and

$$\begin{aligned}
&U(\mathbf{r})=-(U_0\lambda/r)e^{-\lambda r},\quad U_0=2V_0/a_0\lambda\\
&\alpha=f_B(\pi-\theta)/f_B(\theta)=(x^2c^2+1)/(x^2-x^2c^2+1),\\
&T_0(\theta)=\frac{U_0^2\lambda^2}{f_B(\theta)}\left\{\frac{1}{2\pi^2}\int\frac{d\boldsymbol{\eta}}{(\eta^2-k^2)[(\boldsymbol{\eta}-\mathbf{k}_i)^2+\lambda^2][(\boldsymbol{\eta}-\mathbf{k}_s)^2+\lambda^2]}\right\}\\
&\qquad=U_0(1+x^2c^2)\left\{\frac{2}{xcD}\left[\arctan\left(\frac{xc}{D}\right)+\frac{i}{2}\ln\frac{D+x^2c}{D-x^2c}\right]\right\},\\
&D^2=4+4x^2+x^4c^2,
\end{aligned} \tag{14}$$

[5] See reference 4, p. 1149.

where $a_0=\hbar^2/mc^2$ is the first Bohr radius for hydrogen. Upon applying (8) to (12) and solving the resultant equations for C_0 and C_1, we find

$$\begin{aligned} C_0&=\{[1-T_0(\theta)]-\alpha^2[1-T_0(\pi-\theta)]\}/\\ &\quad\{[1-T_0(\theta)]^2-\alpha^2[1-T_0(\pi-\theta)]^2\},\\ C_1&=\alpha\{[1-T_0(\theta)]-[1-T_0(\pi-\theta)]\}/\\ &\quad\{[1-T_0(\theta)]^2-\alpha^2[1-T_0(\pi-\theta)]^2\}. \end{aligned} \tag{15}$$

Hence, upon substitution of these expressions into (12), we find that the scattering amplitude is given by

$$[f_7(\theta)]=f_B(\theta)\frac{(\alpha^2+1)[1-T_0(\theta)]-2\alpha^2[1-T_0(\pi-\theta)]}{[1-T_0(\theta)]^2-\alpha^2[1-T_0(\pi-\theta)]^2}, \tag{16}$$

which at $\theta=\pi/2$ reduces to

$$[f_7(\pi/2)]=f_B(\pi/2)\frac{1}{1-T_0(\pi/2)}. \tag{17}$$

The following stationary values of the scattering amplitude $[f(\theta)]$ for the various trial wave functions listed in (9) were obtained:

$$\begin{aligned}
&\phi_{i1}:\ f_B(\theta)\left\{\frac{1}{1-T_0(\theta)}\right\},\\
&\phi_{i2}:\ f_B(\theta)\left\{\frac{d_0^2[1-T_0(\theta)]-2d_0(d_0-T_1)+(d_1-T_2)}{[1-T_0(\theta)](d_1-T_2)-(d_0-T_1)^2}\right\},\\
&\phi_{i3}:\ f_B(\theta)\left\{\frac{d_2[1-T_0(\theta)]+(d_4-T_4)-2d_2(d_2-T_3)}{[1-T_0(\theta)](a_4-T_4)-(a_2-T_3)^2}\right\},\\
&\phi_{i4'}:\ f_B(\theta)\left\{\frac{d_2[1-T_0(\theta)]+(d_4-T_4)-2d_2(d_2-T_3)}{[1-T_0(\theta)](d_4-T_4)-(d_2-T_3)^2}\right\}+f_B(\theta)\frac{\cos\theta}{d_5-T_6}\left\{d_3-(d_3-T_5)\frac{[(d_4-T_4)-d_2(d_2-T_3)]}{[1-T_0(\theta)](d_4-T_4)-(d_2-T_3)^2}\right\}^2,\\
&\phi_{i5}:\ f_B(\theta)\left\{\frac{d_6^2}{d_6-T_7}+\frac{(1-d_6)^2}{[1-T_0(\theta)]-(d_6-T_7)}\right\},\\
&\phi_{i6}:\ f_B(\theta)\left\{\frac{d_6^2}{d_6-T_7}+\frac{3d_7^2\cos\theta}{d_7-T_8}+\frac{(1-d_6-3d_7\cos\theta)^2}{[1-T_0(\theta)]-(d_6-T_7)-3(d_7-T_8)\cos\theta}\right\},\\
&\phi_{i7}:\ f_B(\theta)\left\{\frac{(\alpha^2+1)[1-T_0(\theta)]-2\alpha^2[1-T_0(\pi-\theta)]}{[1-T_0(\theta)]^2-\alpha^2[1-T_0(\pi-\theta)]^2}\right\},\\
&\phi_{i8}:\ f_B(\theta)\left\{\frac{2(\alpha-d_6)(1-d_6)}{[1-T_0(\theta)]+\alpha[1-T_0(\pi-\theta)]-2(d_6-T_7)}\right.\\
&\qquad\left.+\frac{(1-\alpha^2)\{(d_6-T_7)-[1-T_0(\theta)]\}}{\{\alpha[1-T_0(\pi-\theta)]-[1-T_0(\theta)]\}\{[1-T_0(\theta)]+\alpha[1-T_0(\pi-\theta)]-2(d_6-T_7)\}}+\frac{d_6^2}{d_6-T_7}\right\},\\
&\phi_{i9'}:\ f_B(\theta)\left\{\frac{(\alpha^2+1)[1-T_0(\theta)]-2\alpha^2[1-T_0(\pi-\theta)]}{[1-T_0(\theta)]^2-\alpha^2[1-T_0(\pi-\theta)]^2}\right\}+f_B(\theta)(d_6-T_7)\left\{\frac{d_6}{d_6-T_7}-\frac{1+\alpha}{1-T_0(\theta)+\alpha[1-T_0(\pi-\theta)]}\right\}^2.
\end{aligned} \tag{18}$$

The definitions of the symbols used are included in the Appendix. For two of the trial wave functions ($\phi_{i4'}$ and $\phi_{i9'}$) we have determined the value of the constant C_2 by (8) while taking for the values of C_0 and C_1 those of the previous wave functions (ϕ_{i3} and ϕ_{i8}). To denote this procedure, we insert a prime next to the number of the trial wave function.

Numerical calculations were performed for the differential scattering cross section $|[f(\theta)]|^2$ for each of the algebraic expressions listed in (18); these were then compared with a numerical solution obtained by phase shift analysis. The values of the parameters U_0, λ, and x were taken as

$$\begin{aligned} U_0&=3V_0/4=5.85,\\ \lambda&=8/3a_0,\\ x&=1.44, \end{aligned} \tag{19}$$

where a_0 designates the first Bohr radius for the hydrogen atom. (These values were chosen for future reference for the elastic scattering of electrons from neon.) By numerical solution of the appropriate radial wave equation,[6] the following phase shifts were obtained:

δ_0	δ_1	δ_2	δ_3
188.0°	50.9°	6.3°	1.2°

(The phase shift δ_3 was calculated by a first Born approximation.[7])

Inasmuch as $|f(\theta)|^2$ was expected to be a relatively smooth function of θ, numerical expressions for each of the functions listed in (18) were calculated for only three values of θ: 0, $\frac{1}{2}\pi$, and π. The following numerical values were obtained for the differential scattering cross section, $|[f(\theta)]|^2/a_0^2$, for the various trial wave functions listed:

θ	Num. soln.	ϕ_1	ϕ_2	ϕ_3	$\phi_{4'}$	ϕ_5	ϕ_6	ϕ_7	ϕ_8	$\phi_{9'}$
0	2.41	2.58	0.92	5.31	4.49	2.12	2.14	2.39	2.45	2.42
$\frac{1}{2}\pi$	0.005	0.17	0.03	0.13	0.13	0.28	0.28	0.17	0.28	0.17
π	1.05	0.04	0.15	0.05	0.28	0.29	0.33	1.01	0.47	0.99

From and inspection of the above table we see that the values of $|[f(\theta)]|^2$ at $x=1.44$ associated with ϕ_7 and $\phi_{9'}$ are comparable and, for the trial wave functions chosen, have the "best form." We note that ϕ_7 is the simpler of these two trial wave functions.

ACKNOWLEDGMENTS

The writer is grateful to Professor Philip M. Morse for suggesting the problem and for his understanding and helpful guidance.

APPENDIX. TABULATION OF VARIOUS INTEGRALS

The definitions of the functions d_n, α, and $f_B(\theta)$ which arise from the first three integrals in (6) are as follows:

$$d_0=-\frac{1}{4\pi f_B(\theta)}\int e^{i(\mathbf{k}_i-\mathbf{k}_s)\cdot\mathbf{r}}e^{-\lambda r}U(\mathbf{r})d\mathbf{r}=\frac{x^2c^2+1}{x^2c^2+4},$$

$$d_1=-\frac{1}{4\pi f_B(\theta)}\int e^{i(\mathbf{k}_i-\mathbf{k}_s)\cdot\mathbf{r}}e^{-2\lambda r}U(\mathbf{r})d\mathbf{r}=\frac{x^2c^2+1}{x^2c^2+9},$$

$$d_2=-\frac{1}{4\pi f_B(\theta)}\int e^{i\mathbf{k}_i\cdot\mathbf{r}}e^{-\lambda r}U(\mathbf{r})d\mathbf{r}=\frac{4(x^2c^2+1)}{x^2+16},$$

$$d_3=-\frac{i\lambda}{4\pi f_B(\theta)\cos\theta}\int e^{i\mathbf{k}_i\cdot\mathbf{r}}e^{-\lambda r/2}U(\mathbf{r})(\mathbf{n}_s\cdot\mathbf{r})d\mathbf{r}=\frac{16x(x^2c^2+1)}{(9+x^2)^2},$$

$$d_4=-\frac{1}{4\pi f_B(\theta)}\int e^{-2\lambda r}U(\mathbf{r})d\mathbf{r}=\frac{x^2c^2+1}{9},$$

$$d_5=-\frac{\lambda^2}{12\pi f_B(\theta)}\int e^{-\lambda r}U(\mathbf{r})r^2d\mathbf{r}=\frac{x^2c^2+1}{8},$$

$$d_6=-\frac{1}{4\pi f_B(\theta)}\int e^{i\mathbf{k}_i\cdot\mathbf{r}}U(\mathbf{r})j_0(kr)d\mathbf{r}=\frac{x^2c^2+1}{x^2}\ln(1+x^2),$$

$$d_7=-\frac{i}{4\pi f_B(\theta)\cos\theta}\int e^{i\mathbf{k}_i\cdot\mathbf{r}}U(\mathbf{r})j_1(kr)(\mathbf{n}_s\cdot\mathbf{r})d\mathbf{r}=\frac{2(x^2c^2+1)}{x^2}Q_1\left(1+\frac{2}{x^2}\right),$$

$$f_B(\theta)=-\frac{1}{4\pi}\int U(\mathbf{r})e^{i(\mathbf{k}_i-\mathbf{k}_s)\cdot\mathbf{r}}d\mathbf{r}=\frac{U_0}{\lambda}\frac{1}{x^2c^2+1},$$

$$\alpha=\frac{f_B(\pi-\theta)}{f_B(\theta)}=\frac{x^2c^2+1}{x^2(1-c^2)+1},$$

$$U(\mathbf{r})=-U_0(\lambda/r)e^{-\lambda r},\quad x=2k/\lambda,\quad c=\sin(\theta/2),$$

$$Q_1(z)=\tfrac{1}{2}z\ln\left(\frac{z+1}{z-1}\right)-1,\quad z>1.$$

The evaluation of the double integral which occurs in (6) is simplified by a transformation to momentum space; thus, the Green function is replaced by its Fourier transform

$$G(\mathbf{r},\mathbf{r}')=\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}=\frac{4\pi}{(2\pi)^3}\int\frac{d\boldsymbol{\eta}\exp[i\boldsymbol{\eta}\cdot(\mathbf{r}-\mathbf{r}')]}{\eta^2-k^2},\qquad\text{(A.1)}$$

where the path of integration is defined to be over the pole at $\eta=-k$ and under that at $+k$. Hence, double integrals of the form

$$\iint J_1(\mathbf{r},-\mathbf{k}_s)G(\mathbf{r},\mathbf{r}')J_2(\mathbf{r}',\mathbf{k}_i)d\mathbf{r}d\mathbf{r}'\qquad\text{(A.2)}$$

are reduced to integrals of the form

$$4\pi\int\frac{d\boldsymbol{\eta}}{\eta^2-k^2}K_1(\boldsymbol{\eta},-\mathbf{k}_s)K_2(-\boldsymbol{\eta},\mathbf{k}_i),$$
$$K(\boldsymbol{\eta},\mathbf{k})=(2\pi)^{-\frac{3}{2}}\int J(\mathbf{r},\mathbf{k})e^{i\boldsymbol{\eta}\cdot\mathbf{r}}d\mathbf{r}.\qquad\text{(A.3)}$$

In several of the double integrals the resultant algebraic expressions are simplified if, prior to integration, a coordinate transformation is carried out[8] or Feynman's method[9] of grouping factors is used.

Thus, the definitions of the functions $T_n(\theta)$, which

[6] See reference 3, p. 129.

[7] See reference 3, pp. 28 and 119.

[8] G. Källén, Arkiv Fysik **2**, 33 (1950).

[9] R. H. Dalitz, Proc. Roy. Soc. (London) **A206**, 509 (1950).

arise from the double integral in (6) are as follows:

$$T_0(\theta,x)=\frac{U_0{}^2\lambda^2}{2\pi^2 f_B(\theta)}\int\frac{d\boldsymbol{\eta}}{(\eta^2-k^2)[(\boldsymbol{\eta}-\mathbf{k}_i)^2+\lambda^2][(\boldsymbol{\eta}-\mathbf{k}_s)^2+\lambda^2]}=\left(\frac{U_0{}^2}{\lambda f_B(\theta)}\right)\frac{2}{xcD}\left[\tan^{-1}\frac{xc}{D}+\frac{i}{2}\ln\frac{D+x^2c}{D-x^2c}\right],$$

$$T_1(\theta)=\frac{U_0{}^2\lambda^2}{2\pi^2 f_B(\theta)}\int\frac{d\boldsymbol{\eta}}{(\eta^2-k^2)[(\boldsymbol{\eta}-\mathbf{k}_i)^2+4\lambda^2][(\boldsymbol{\eta}-\mathbf{k}_s)^2+\lambda^2]}=\left(\frac{U_0{}^2}{\lambda f_B(\theta)}\right)\frac{1}{xb_1}\left\{\left[\tan^{-1}\frac{xb_1}{3-x^2c^2}-\tan^{-1}\frac{xb_1}{2(3+x^2c^2)}\right]\right.$$
$$\left.+\frac{i}{2}\ln\left[\frac{16b_2{}^2+x^2(b_3+b_1)^2}{16b_2{}^2+x^2(b_3-b_1)^2}\right]\cdot\left[\frac{4b_2{}^2+x^2(b_4+b_1)^2}{4b_2{}^2+x^2(b_4-b_1)^2}\right]\right\},$$

$$T_2(\theta)=\frac{x^2c^2+1}{2(x^2c^2+4)}T_0(\theta,x/2),$$

$$T_3(\theta)=\frac{U_0{}^2\lambda^2}{2\pi^2 f_B(\theta)}\int\frac{d\boldsymbol{\eta}}{(\eta^2-k^2)[(\boldsymbol{\eta}-\mathbf{k}_i)^2+\lambda^2][\eta^2+4\lambda^2]}=\left(\frac{U_0{}^2}{\lambda f_B(\theta)}\right)\frac{4}{x(x^2+16)}\left[\tan^{-1}x-2\tan^{-1}\frac{x}{6}+\frac{i}{2}\ln(1+x^2)\right],$$

$$T_4(\theta)=\frac{U_0{}^2\lambda^2}{2\pi^2 f_B(\theta)}\int\frac{d\boldsymbol{\eta}}{(\eta^2-k^2)(\eta^2+4\lambda^2)^2}=\left(\frac{U_0{}^2}{\lambda f_B(\theta)}\right)\left[\frac{16-x^2+i8x}{(16+x^2)^2}\right],$$

$$T_5(\theta)=\frac{U_0{}^2\lambda^3}{4\pi^2 f_B(\theta)\cos\theta}\int\frac{\mathbf{n}_s\cdot\boldsymbol{\eta}\,d\boldsymbol{\eta}}{(\eta^2-k^2)(\eta^2+9\lambda^2/4)^2[(\mathbf{k}_i-\boldsymbol{\eta})^2+\lambda^2]}$$
$$=-\left(\frac{U_0{}^2}{\lambda f_B(\theta)}\right)\frac{4}{x(x^2+9)^2}\left\{i\left[x-\frac{2+x^2}{2x}\ln(1+x^2)\right]+\frac{2(15-x^2)}{25+x^2}+\frac{(2+x^2)}{x}[2\tan^{-1}(x/5)-\tan^{-1}x]\right\},$$

$$T_6(\theta)=\frac{U_0{}^2\lambda^4}{8\pi^2 f_B(\theta)\cos\theta}\int\frac{(\mathbf{n}_s\cdot\boldsymbol{\eta})(\mathbf{n}_i\cdot\boldsymbol{\eta})d\boldsymbol{\eta}}{(\eta^2-k^2)(\eta^2+9\lambda^2/4)^4}=\left(\frac{U_0{}^2}{\lambda f_B(\theta)}\right)\frac{1}{3(9+x^2)^4}\left[i8x^3-\frac{(x^6+81x^4-729x^2-729)}{54}\right],$$

$$T_7(\theta)=\frac{U_0{}^2}{8\pi^2x^2 f_B(\theta)}\int\frac{d\boldsymbol{\eta}}{\eta^2(\eta^2-k^2)}\left\{\ln\frac{(\eta+k)^2+\lambda^2}{(\eta-k)^2+\lambda^2}\right\}^2=\left(\frac{U_0{}^2}{\lambda f_B(\theta)}\right)\frac{2}{x^3}\left\{\frac{i}{4}[\ln(1+x^2)]^2\right.$$
$$\left.+(\tfrac{1}{2}\pi-\tan^{-1}x)\ln(1+x^2)+\sum_{n=1}^{\infty}\frac{\sin(2n\tan^{-1}x)}{n^2(1+x^2)^n}-\sum_{n=1}^{\infty}\frac{\sin(2n\tan^{-1}x)}{n^2}\right\},$$

$$T_8(\theta)=\frac{U_0{}^2}{2\pi^2x^2 f_B(\theta)}\int\frac{d\boldsymbol{\eta}}{\eta^2(\eta^2-k^2)}\left[Q_1\left(\frac{\lambda^2+k^2+\eta^2}{2k\eta}\right)\right]^2=\left(\frac{U_0{}^2}{\lambda f_B(\theta)}\right)\frac{2}{x^3}\left\{i\left[Q_1\left(\frac{2+x^2}{x^2}\right)\right]^2\right.$$
$$+\frac{4}{x^3}\ln\left(1+\frac{x^2}{4}\right)-2\left(\frac{x^2+2}{x^2}\right)\tan^{-1}\left(\frac{x}{2+x^2}\right)$$
$$\left.+\left(\frac{2+x^2}{x^2}\right)^2\left[\left(\frac{\pi}{2}-\tan^{-1}x\right)\ln(1+x^2)+\sum_{n=1}^{\infty}\frac{\sin(2n\tan^{-1}x)}{n^2(1+x^2)^n}-\sum_{n=1}^{\infty}\frac{\sin(2n\tan^{-1}x)}{n^2}\right]\right\},$$

$$c=\sin(\theta/2),\qquad b_1{}^2=(x^2c^2+5)^2+16c^2-16,$$
$$x=2k/\lambda,\qquad b_2=3-x^2c,$$
$$D^2=4+4x^2+x^4c^2,\qquad b_3=x^2c^2-8c-3,$$
$$Q_1(z)=\tfrac{1}{2}z\ln\left(\frac{z+1}{z-1}\right)-1,\qquad b_4=x^2c^2+2c+3.$$