JOURNAL OF COMPUTATIONAL PHYSICS 6, 237–246 (1970)

# Integrals Involving Continuum Wavefunctions I: One-Center Coulomb Integrals

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Received December 10, 1969; revised February 25, 1970

Integrals required in the application of variational principles to the scattering of electrons by atoms are reviewed, special attention being paid to the case of a coulomb field. A technique is described for the evaluation of integrals involving two continuum functions.

## 1. INTRODUCTION

Increases in the size and speed of computers in recent years have led to an awakened interest in the variational approach to scattering calculations [1]. This approach reduces the problem to one of evaluating one- and two-electron integrals over the orbitals of the chosen basis set. We shall describe rapid and accurate methods of calculating the integrals. The methods are essentially analytical and do not require any numerical tabulations of continuum wavefunctions.

The radial integrals are of five types,

$$I_1 = [a_1 \mid f_1] = \int_0^\infty a_1(r) f_1(r)\, r^2\, dr, \tag{1}$$

$$\begin{aligned} I_2 &= [f_1 \mid T_\lambda \mid f^2] \\ &= \frac{1}{2} \int_0^\infty r f_1(r) \left\{ -\frac{d^2}{dr^2} - k^2 - \frac{Z}{r} + \frac{\lambda(\lambda+1)}{r^2} \right\} r f_2(r)\, dr, \end{aligned} \tag{2}$$

$$\begin{aligned} J_1 &= [a_1 a_2 \mid r_<^\lambda / r_>^{\lambda+1} \mid f_1 a_3] \\ &= \int_0^\infty dr\, r^2 a_1(r) f_1(r) \left\{ r^\lambda \int_r^\infty dr'\, r'^2 a_2(r')\, a_3(r') \Big/ r'^{\lambda+1} \right. \\ &\quad \left. + (1/r^{\lambda+1}) \int_0^r dr'\, r'^2 a_2(r')\, a_3(r')\, r'^\lambda \right\}, \end{aligned} \tag{3}$$

$$J_2 = [f_1 a_1 \mid r_<^{\lambda}/r_>^{\lambda+1} \mid f_2 a_2]$$

$$= \int_0^\infty dr\, r^2 f_1(r) f_2(r) \Big\{ r^\lambda \int_r^\infty dr'\, r'^2 a_1(r')\, a_2(r') \Big/ r'^{\lambda+1}$$

$$+ (1/r^{\lambda+1}) \int_0^r dr\, r'^2 a_1(r')\, a_2(r')\, r'^\lambda \Big\}, \tag{4}$$

$$J_3 = [a_1 f_1 \mid r_<^{\lambda}/r_>^{\lambda+1} \mid f_2 a_2]$$

$$= \int_0^\infty dr\, r^2 a_1(r) f_2(r) \Big\{ r^\lambda \int_r^\infty dr'\, r'^2 a_2(r') f_1(r') \Big/ r'^{\lambda+1}$$

$$+ (1/r^{\lambda+1}) \int_0^r dr'\, r'^2 a_2(r') f_1(r')\, r'^\lambda \Big\}, \tag{5}$$

where $a_1$, $a_2$, $a_3$ are bound state orbitals and $f_1$, $f_2$ are continuum orbitals. If we introduce the Slater orbitals,

$$S_j(r) = r^{n_j - 1} e^{-\zeta_j r}, \tag{6}$$

the bound orbitals may be represented by expansions such as,

$$a(r) \cong \sum_{j=1}^{M} C_j S_j(r). \tag{7}$$

In order to satisfy the boundary condition on a continuum orbital, which always has the form,

$$f(r) \underset{r\to\infty}{\sim} \mathscr{J}_l(\eta, kr) + R\mathscr{N}_l(\eta, kr), \tag{8}$$

we use the fact that

$$\mathscr{N}_l \underset{r\to\infty}{\sim} \left(\frac{\eta}{l+1}\right) \mathscr{J}_l + \left[1 + \left(\frac{\eta}{l+1}\right)^2\right]^{1/2} \mathscr{J}_{l+1} \tag{9}$$

and write,

$$f(r) \cong A\mathscr{J}_l + B\mathscr{J}_{l+1} + \sum_{j=1}^{M} C_j S_j\,. \tag{10}$$

$\mathscr{J}_l$ and $\mathscr{N}_l$ are coulomb–bessel functions defined in 2.[1]

[1] The coulomb–bessel functions are related to the more familiar coulomb functions by the equations, $\mathscr{J}_l(\eta, t) = F_l(\eta, t)/t$, $\mathscr{N}_l(\eta, t) = G_l(\eta, t)/t$.

The integrals (1)–(5) can now be expressed in terms of five standard functions,

$$f_m^l(\eta, k, \alpha) = \int_0^\infty x^m e^{-\alpha x} \mathscr{F}_l(\eta, kx)\, dx, \tag{11}$$

$$f_m^{ll'}(\eta, \eta', k, k', \alpha) = \int_0^\infty x^m e^{-\alpha x} \mathscr{F}_l(\eta, kx)\, \mathscr{F}_{l'}(\eta', k'x)\, dx, \tag{12}$$

$$H_{mn}^l(\eta, k, \alpha, \beta) = \int_0^\infty x^m e^{-\alpha x} \mathscr{F}_l(\eta, kx)\, dx \int_x^\infty y^n e^{-\beta y}\, dy, \tag{13}$$

$$H_{mn}^{ll'}(\eta, \eta', k, k', \alpha, \beta) = \int_0^\infty x^m e^{-\alpha x} \mathscr{F}_l(\eta, kx) \mathscr{F}_{l'}(\eta', k'x)\, dx \int_x^\infty y^n e^{-\beta y}\, dy, \tag{14}$$

$$\bar{H}_{mn}^{ll'}(\eta, \eta', k, k', \alpha, \beta) = \int_0^\infty x^m e^{-\alpha x} \mathscr{F}_l(\eta, kx)\, dx \int_x^\infty y^n e^{-\beta y} \mathscr{F}_{l'}(\eta', k'y)\, dy. \tag{15}$$

## 2. Coulomb Wavefunctions

The radial wavefunction in a coulomb field of effective charge $Z$ satisfies the differential equation (cf. [2], [3]).

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + k^2 + \frac{2Z}{r} - \frac{l(l+1)}{r^2} \right\} \phi(r) = 0. \tag{16}$$

It is convenient to introduce the parameter $\eta$

$$\eta = Z/k. \tag{17}$$

The regular solution of (16) may be expressed as a confluent hypergeometric function ${}_1F_1$. The coulomb–bessel function defined by

$$\mathscr{F}_l(\eta, kr) = \mathscr{C}_l(\eta)\, e^{ikr} (2kr)^l\, {}_1F_1(l + 1 - i\eta;\, 2l + 2;\, -2ikr) \tag{18}$$

is a solution of (16) which we adopt as the standard notation. If $\eta \to 0$ we recover the spherical bessel function,

$$\lim_{\eta \to 0} \mathscr{F}(\eta, kr) = j_l(kr). \tag{19}$$

The normalizing factor $\mathscr{C}_l$ is

$$\begin{aligned} \mathscr{C}_l(\eta) &= e^{\pi\eta/2}\, |\, \Gamma(l + 1 + i\eta)|/2l + 1! \\ &= \frac{1}{2l+1!} \left| \frac{2\pi\eta}{1 - e^{-2\pi\eta}} \prod_{s=1}^{l} (s^2 + \eta^2) \right|^{1/2}. \end{aligned} \tag{20}$$

The asymptotic form of $\mathscr{F}_l(\eta, kr)$ is (cf. [2] p. 541).

$$\mathscr{F}_l(\eta, kr) \underset{r\to\infty}{\sim} \frac{\sin \Theta_l(\eta, kr)}{kr}, \tag{21}$$

where

$$\Theta_l(\eta, kr) = kr + \eta \ln(kr) + \sigma_l - \frac{l\pi}{2}, \tag{22}$$

$$\begin{aligned} \sigma_l &= ph\Gamma(l + 1 - i\eta) \\ &= -\eta\psi(l + 1) + \sum_{s=l+1}^{\infty} \left\{\arctan\left(\frac{\eta}{s}\right) - \left(\frac{\eta}{s}\right)\right\}, \end{aligned} \tag{23}$$

$$\psi(l + 1) = -\gamma + \sum_{s=1}^{l} \frac{1}{s} \qquad (\gamma \text{ is Euler's constant}). \tag{24}$$

The asymptotic behavior of the irregular (logarithmic) solution is given by,

$$\mathscr{N}_l(\eta, kr) \underset{r\to\infty}{\sim} - \frac{\cos \Theta_l(\eta, kr)}{kr}. \tag{25}$$

## 3. The Functions $f_m{}^l(\eta, k, \alpha)$

If we substitute (18) in (11), expand ${}_1F_1$ in a convergent power series, and integrate term by term we find that [4]

$$\begin{aligned} f_m{}^l(\eta, k, \alpha) &= \frac{\overline{l + m}!\,(2k)^l\, \mathscr{C}_l(\eta)}{(\alpha - ik)^{l+m+1}} \left(\frac{\alpha - ik}{\alpha + ik}\right)^{l+1-i\eta} \\ &\cdot {}_2F_1\left(l + 1 - i\eta, l + m + 1; 2l + 2; \frac{2ik}{\alpha + ik}\right) \end{aligned} \tag{26}$$

for $|\,2k\,| \leqslant |\,\alpha + ik\,|$; the function exists for other values by analytic continuation. Transforming ${}_2F_1$ by a well-known theorem [6, p. 64] we obtain

$$f_m{}^l(\eta, k, \alpha) = \frac{\overline{l + m}!\,(2k)^l\, \mathscr{C}_l(\eta)}{(\alpha + ik)^{l+m+1}}\, {}_2F_1\left(l + 1 + i\eta, l + m + 1; 2l + 2; \frac{2ik}{\alpha + ik}\right). \tag{27}$$

Comparing (26) and (27) we find

$$\frac{f^l_{-m}(-\eta, k, \alpha)}{f_m{}^l(\eta, k, \alpha)} = \frac{\overline{l - m}!}{\overline{l + m}!} (k^2 + \alpha^2)^m \exp\{-2\eta \arctan(\alpha/k)\}. \tag{28}$$

While (26) is not suitable for direct computation it can be used to derive expressions for $f_m{}^l$ in special cases. If $m = l + 1$ we have

$$f_{l+1}^{l}(\eta, k, \alpha) = \frac{2l + 1!\,(2k)^l\,\mathscr{C}_l(\eta)}{(k^2 + \alpha^2)^{l+1}} \exp\{-2\eta \arctan(k/\alpha)\}. \tag{29}$$

Since $f_0{}^0(\eta, k, \alpha) = \int_\alpha^\infty f_1{}^0(\eta, k, t)\,dt$, or using the series directly, it is readily shown that

$$f_0{}^0(\eta, k, \alpha) = \frac{\mathscr{C}_0(\eta)}{2\eta k}\{1 - \exp[-2\eta \arctan(k/\alpha)]\}. \tag{30}$$

We compute the other $f_m{}^l$ by means of recurrence relations, starting with the recurrence relations [2] satisfied by the coulomb–bessel functions $\mathscr{J}_l(\eta, x)$,

$$\left[1 + \left(\frac{\eta}{l+1}\right)^2\right]^{1/2} \mathscr{J}_{l+1} - (2l+1)\left[\frac{1}{x} - \frac{\eta}{l(l+1)}\right]\mathscr{J}_l + \left[1 + \left(\frac{\eta}{l}\right)^2\right]^{1/2} \mathscr{J}_{l-1} = 0, \tag{31}$$

$$(2l+1)\frac{d}{dx}\mathscr{J}_l = l\left[1 + \left(\frac{\eta}{l}\right)^2\right]^{1/2}\mathscr{J}_{l-1} - (l+1)\left[1 + \left(\frac{\eta}{l+1}\right)^2\right]^{1/2}\mathscr{J}_{l+1}. \tag{32}$$

From (31) we deduce

$$\left[1 + \left(\frac{\eta}{l+1}\right)^2\right]^{1/2} f_l^{l+1} - \frac{(2l+1)}{k}\left[f_{m-1}^{l} - \frac{k\eta}{l(l+1)} f_m{}^l\right] + \left[1 + \left(\frac{\eta}{l}\right)^2\right] f_m^{l-1} = 0, \tag{33}$$

and from (32)

$$l\left[1 + \left(\frac{\eta}{l}\right)^2\right]^{1/2} f_m^{l-1} - (l+1)\left[1 + \left(\frac{\eta}{l+1}\right)^2\right]^{1/2} f_m^{l+1} = \frac{(2l+1)}{k}(\alpha f_m{}^l + m f_{m-1}^{l}) \qquad (l + m \mid > 0). \tag{34}$$

Eliminating $f_{m-1}^{l}$ between (33) and (34) we have

$$(l - m + 1)\left[1 + \left(\frac{\eta}{l+1}\right)^2\right]^{1/2} f_m^{l+1} + (2l+1)\left[\frac{\alpha}{k} - \frac{m\eta}{l(l+1)}\right] f_m{}^l - (l+m)\left[1 + \left(\frac{\eta}{l}\right)^2\right]^{1/2} f_m^{l-1} = 0 \qquad (l + m \mid > 0). \tag{35}$$

The case $l = m = 0$ must be examined separately,

$$(1 + \eta^2)^{1/2} f_0^1 + \left(\frac{\alpha}{k} + \eta\right) f_0^0 = \frac{\mathscr{C}_0(\eta)}{k}. \tag{36}$$

The relationship

$$(k^2 + \alpha^2) f_{m+1}^l - 2(m\alpha - k) f_m{}^l - (l + m)(l - m + 1) f_{m-1}^l = 0 \tag{37}$$

was derived by Bransden and Dalgarno [5] directly from the differential equation (16). It may be obtained from (33) and (34) with a great deal of effort. From (34) and (35) we obtain

$$\left[1 + \left(\frac{\eta}{l}\right)^2\right]^{1/2} f_{l+1}^{l+1} - \frac{(2l+1)}{k} f_l{}^l + \left[\frac{\alpha}{k} + \frac{\eta}{(l+1)}\right] f_{l+1}^l = 0. \tag{38}$$

Finally from (33) and (34) we have

$$\frac{(l - m + 1)}{\alpha} f_{m-1}^l = \left[1 + \left(\frac{\eta}{l}\right)^2\right]^{1/2} f_m^{l-1} - \left(\frac{\alpha}{k} - \frac{\eta}{l}\right) f_m{}^l. \tag{39}$$

We now outline an algorithm for computing $f_m{}^l(\eta, k, \alpha)$ where $l = 0(1)l_{\text{MAX}}$ and $m = -l(1)m_{\text{MAX}}$. Equation (29) is used to evaluate $f_{l+1}^l$ for $l = 0, 1,...,$ $\max(l_{\text{MAX}}, m_{\text{MAX}} - 1)$; then (38) is used to obtain $f_l{}^l$ for $l = 0, 1,...,$ $\max(l_{\text{MAX}}, m_{\text{MAX}})$ starting from (30); (35) gives $f_l^{l+\delta}$ for $\delta = 1, 2,..., l_{\text{MAX}} - 1$ and $f_l^{l-\delta}$ for $\delta = 2, 3,..., l$; finally $f_{-m}^l$ for $m = 1, 2,..., l$ is calculated using (39). If only a single value of $l$ occurs it is more convenient to make use of (37). $f_m{}^l$ may be evaluated for a negative $m$ using (28); however if the value of $f_{|m|}^l$ is also required this procedure necessitates the calculation of both $f_{|m|}^l(\eta, k, \alpha)$ and $f_{|m|}^l(-\eta, k, \alpha)$ and so it is not recommended unless $\eta = 0$.

## 4. The Functions $f_m^{ll'}(\eta, \eta', k, k', \alpha)$ and $H_m^{ll'}(\eta, \eta', k, k', \alpha, \beta)$

To handle integrals involving the product of two coulomb wavefunctions we use the following integral representation [2],

$$\mathscr{F}_l(\eta, x) = \frac{e^{\pi\eta} x^l}{2l + 1!\, \mathscr{C}_l(\eta)\, 2^{l+1}} \int_{-\infty}^{+\infty} (1 - \tanh^2 u)^{l+1} \exp i(x \tanh u + 2\eta u)\, du. \tag{40}$$

Thus, transforming the function $\mathscr{F}_l$ in (12) by means of (40), we obtain the expression

$$f_m^{ll'}(\eta, \eta', k, k', \alpha)$$
$$= \frac{2e^{\pi\eta}(2k)^l}{2l + 1!\, \mathscr{C}_l(\eta)} \int_{-\infty}^{+\infty} \frac{e^{-2(l+1-i\eta)u}}{(1 + e^{-2u})^{2l+2}} f_{m+l}^{l'}(\eta', k', \alpha - ik \tanh u)\, du. \tag{41}$$

The integral in (41) may be evaluated using a Gauss–Laguerre quadrature formula. The methods of calculating $f_m(\eta, k, \alpha)$ described in [3] are equally applicable for complex values of $\alpha$ (Re $\alpha \geqslant 0$).

By the same reasoning we can express the integral $\tilde{H}_{mn}^{ll'}$, defined by (15), in the form

$$\tilde{H}_{mn}^{ll'}(\eta, \eta', k, k', \alpha, \beta)$$
$$= \frac{2e^{\pi\eta}(2k)^l}{2l+1!\,\mathscr{C}_l(\eta)} \int_{-\infty}^{+\infty} \frac{e^{-2(l+1-i\eta)u}}{(1+e^{-2u})^{2l+2}} H_{m+ln}^{l'}(\eta', k', \alpha, \beta - ik\tanh u)\, du. \tag{42}$$

The evaluation of $H_{mn}^l$ is described in Section 5.

In a few special cases $f_m^{ll'}$ may be evaluated in closed forms. Since these special cases are useful as numerical checks they are included in an Appendix.

## 5. The Integrals $H_{mn}^l(\eta, k, \alpha, \beta)$ and $H_{mn}^{ll'}(\eta, \eta', k, k', \alpha, \beta)$

Consider the integrals of the general form

$$\Phi_{mn}(\alpha, \beta) = \int_0^\infty x^m e^{-\alpha x} \varphi(x)\, dx \int_x^\infty y^n e^{-\beta y}\, dy. \tag{43}$$

Repeated integration by parts gives the result

$$\Phi_{mn}(\alpha, \beta) = \frac{n!}{\beta^n} \sum_{s=0}^{\infty} \frac{\beta^s}{s!} \Psi_{m+s}(\alpha+\beta), \tag{44}$$

where

$$\Psi_q(\gamma) = \int_0^\infty x^q e^{-\gamma x} \varphi(x)\, dx. \tag{45}$$

An economical way to compute $\Phi_{mn}$ is to use the recurrence relation

$$\Phi_{mn}(\alpha, \beta) = \frac{1}{\beta} \Psi_{m+n}(\alpha+\beta) + \frac{n}{\beta} \Phi_{mn-1}(\alpha, \beta). \tag{46}$$

As special cases of (46) we have

$$\begin{aligned} H_{mn}^l(\eta, k, \alpha, \beta) &= \frac{1}{\beta} f_{m+n}^l(\eta, k, \alpha+\beta) + \frac{n}{\beta} H_{mn-1}^l(\eta, k, \alpha, \beta), \\ H_{mn}^{ll'}(\eta, \eta', k, k', \alpha, \beta) &= \frac{1}{\beta} f_{m+n}^{ll'}(\eta, \eta', k, k', \alpha+\beta) + \frac{n}{\beta} H_{mn-1}^{ll'}(\eta, \eta', k, k', \alpha, \beta). \end{aligned} \tag{47}$$

## 6. Conclusion

Experience has shown that the methods described in this paper are highly suitable for automatic computation. Special results involving the spherical bessel functions (19) may be obtained by putting $\eta, \eta' = 0$ everywhere.[2]

## APPENDIX: Closed Formulas for $f_m^{ll'}$

The following very general theorem may be proved using integral representations of the hypergeometric functions,

$$\int_0^\infty x^\nu e^{-\mu x} {}_1F_1(a; c; \lambda x)\, {}_1F_1(a'; c'; \lambda' x)\, dx$$

$$= \frac{\Gamma(c)\, \Gamma(c')\, \Gamma(\nu + 1)}{\Gamma(a)\, \Gamma(c - a)\, \Gamma(a')\, \Gamma(c' - a')\, \mu^{\nu+1}} \mathbf{F}_2(\nu + 1, a, a', c, c', \lambda/\mu, \lambda'/\mu') \quad (49)$$

where $\mathbf{F}_2$ is the hypergeometric function of two variables [6]. If we use Eq. (18) to express the coulomb–bessel functions in terms of ${}_1F_1$, (49) gives the result,

$$f_m^{ll'}(\eta, \eta', k, k', \alpha)$$

$$= \frac{l + l' + m!\, (2k)^l\, (2k')^{l'} \exp \tfrac{1}{2}\pi(\eta + \eta')}{|\, \Gamma(l + 1 + i\eta)\, \Gamma(l' + 1 + i\eta')|\, [\alpha + i(k + k')]^{l+l'+m+1}}$$

$$\cdot\, \mathbf{F}_2(l' + l + m + 1, l + 1 + i\eta, l' + 1 + i\eta', 2l + 2, 2l' + 2,$$

$$2ik/[\alpha + i(k + k')], 2ik'/[\alpha + i(k + k')]). \quad (50)$$

If $c = c'$ in (49), the integral is expressible as an ordinary hypergeometric function [6, p. 287],

$$\int_0^\infty x^\nu e^{-\mu x} {}_1F_1(a; c; \lambda x)\, {}_1F_1(a'; c; \lambda' x)\, dx$$

$$= \frac{\Gamma(c)\, \mu^{a+a'-c}}{(\mu - \lambda)^a\, (\mu - \lambda')^{a'}}\, {}_2F_1 \left[a, a'; c; \frac{\lambda\lambda'}{(\mu - \lambda)(\mu - \lambda')}\right]. \quad (51)$$

[2] Lyons and Nesbet [8] have independently devised procedures for integrals containing spherical bessel functions. Their method for the $f_m{}^l$ integrals is similar to that used in the present paper, but they approach the $f_m^{ll'}$ integrals in a very different way. I am grateful to Dr. Nesbet for sending me his work in advance of publication.

$$f^{ll}(\eta, \eta', k, k', \alpha)$$
$$= \frac{2l+m!\,(4kk')^l \exp \tfrac{1}{2}\pi(\eta+\eta')\,|\,\Gamma(l+1+i\eta)\,\Gamma(l+1-i\eta')|}{(2l+1!)^2\,(\alpha-ik+ik')^{l+1+i\eta}\,(\alpha+ik-ik')^{l+1+i\eta'}}$$
$$\cdot\, {}_2F_1\left[l+1+i\eta, l+1+i\eta'; 2l+2; \frac{-4kk'}{\alpha^2+(k-k')^2}\right] \qquad (\mathrm{Re}\,\alpha > 0). \quad (52)$$

These formulas are not convenient for computation.

By using relations derived for bessel functions [7] it may be shown that

$$f_m^{ll'}(0, 0, k, k, 2\alpha)$$
$$\frac{k^{l+l'}l+l'+m!}{2^{l+l'+m}l+l'+1!}\int_0^{\pi/2}\frac{(\cos\Phi)^{l+l'+1}\cos(l-l')\Phi}{(\alpha^2+k^2\cos^2\Phi)^{(l+l'+m+1)/2}}{}_2F_1[(l+l'+m+1)/2,$$
$$(l+l'-m+2)/2, l+l'+2, (k^2\cos^2\Phi)/(\alpha^2+k^2\cos^2\Phi)]\,d\Phi, \qquad (53)$$

which is more simply written as

$$f_m^{ll'}(0, 0, k, k, 2\alpha)$$
$$= \left(\frac{8\pi}{k}\right)^{1/2}\left(\frac{1}{2}\right)^m \int_0^{\pi/2}(\cos\Phi)^{1/2}\cos(l-l')\,\Phi f_{m-1/2}^{l+l'+1/2}(0, k\cos\Phi, 0)\,d\Phi. \quad (54)$$

These formulas do not appear to be more than curiosities.

From the differential equation (16) we can show that

$$f_0^{ll'}(\eta, \eta, k, k, 0) = \frac{\sin[(l-l')\pi/2-(\sigma_l-\sigma_{l'})]}{k(l-l')(l+l'+1)} \qquad (55)$$

where $\sigma_l$ is defined by (23). If $l' > l$ (51) becomes

$$f_0^{ll'}(\eta, \eta, k, k, 0) = \frac{\sin[(l-l')\pi/2-\sum_{s=l+1}^{l'}\arctan(\eta/s)]}{k(l-l')(l+l'+1)} \qquad (56)$$

But if we let $l \to l'$ in (51) we have

$$\begin{aligned} f_0^{ll}(\eta, \eta, k, k, 0) &= \frac{1}{k(2l+1)}\left(\frac{\pi}{2}-\frac{\partial\sigma_l}{\partial l}\right) \\ &= \frac{\pi}{2k(2l+1)}+\frac{\eta}{(2l+1)}\sum_{s=l+1}^{\infty}\frac{1}{(s^2+\eta^2)}. \end{aligned} \qquad (57)$$

The infinite summation in (5) can be evaluated exactly, since

$$\sum_{s=1}^{\infty}\frac{1}{(s^2+\eta^2)} = \frac{1}{2\eta^2}\left\{\frac{2\pi\eta}{e^{2\pi\eta}-1}+\pi\eta-1\right\}. \qquad (58)$$

## Acknowledgments

I should like to thank Professor A. Dalgarno and Professor J. C. Browne for their encouragement of this work which was supported by the Air Force Office of Scientific Research, Office of Aerospace Research, United States Air Force, under AFOSR Grant NR69-1731.

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