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Citation Details
Straton, J.C. Integral Representations over Finite Limits for Quantum Amplitudes. Axioms 2024, 13, 120.
https://doi.org/10.3390/ axioms13020120

axioms

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Integral Representations over Finite Limits for Quantum Amplitudes

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Abstract: We extend previous research to derive three additional M-1-dimensional integral representations over the interval $[0,1]$. The prior version covered the interval $[0,\infty]$. This extension applies to products of M Slater orbitals, since they (and wave functions derived from them) appear in quantum transition amplitudes. It enables the magnitudes of coordinate vector differences (square roots of polynomials) $|\mathbf{x}_1 - \mathbf{x}_2| = \sqrt{x_1^2 - 2x_1x_2\cos\theta + x_2^2}$ to be shifted from disjoint products of functions into a single quadratic form, allowing for the completion of its square. The M-1-dimensional integral representations of M Slater orbitals that both this extension and the prior version introduce provide alternatives to Fourier transforms and are much more compact. The latter introduce a 3M-dimensional momentum integral for M products of Slater orbitals (in M separate denominators), followed in many cases by another set of M-1-dimensional integral representations to combine those denominators into one denominator having a single (momentum) quadratic form. The current and prior methods are also slightly more compact than Gaussian transforms that introduce an M-dimensional integral for products of M Slater orbitals while simultaneously moving them into a single (spatial) quadratic form in a common exponential. One may also use addition theorems for extracting the angular variables or even direct integration at times. Each method has its strengths and weaknesses. We found that these M-1-dimensional integral representations over the interval $[0,1]$ are numerically stable, as was the prior version, having integrals running over the interval $[0,\infty]$, and one does not need to test for a sufficiently large upper integration limit as one does for the latter approach. For analytical reductions of integrals arising from any of the three, however, there is the possible drawback for large M of there being fewer tabled integrals over $[0,1]$ than over $[0,\infty]$. In particular, the results of both prior and current representations have integration variables residing within square roots asarguments of Macdonald functions. In a number of cases, these can be converted to Meijer G-functions whose arguments have the form $(ax^2+bx+c)/x$, for which a single tabled integral exists for the integrals from running over the interval $[0,\infty]$ of the prior paper, and from which other forms can be found using the techniques given therein. This is not so for integral representations over the interval $[0,1]$. Finally, we introduce a fourth integral representation that is not easily generalizable to large M but may well provide a bridge for finding the requisite integrals for such Meijer G-functions over $[0,1]$.

Keywords: integral transform; integral representation; quantum amplitudes; integrals of Macdonald functions; integrals of hypergeometric functions; integrals of Meijer G-functions; Feynman integrals

MSC: 44A20; 44A30; 81Q30; 81Q99; 33C10; 33C70; 33C60

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Citation: Straton, J.C. Integral Representations over Finite Limits for Quantum Amplitudes. *Axioms* **2024**, *13*, 120. https://doi.org/10.3390/axioms13020120

Academic Editor: Hari Mohan Srivastava

Received: 3 January 2024
Revised: 2 February 2024
Accepted: 8 February 2024
Published: 14 February 2024

1. Introduction

When evaluating quantum transition amplitudes, one is faced with the analytical reduction of integrals involving explicit functions of the interelectron (or nucleon) distances. On occasion, one can integrate them directly (see, for instance, [1], among many others), while at other times, addition theorems (e.g., [2–4]) are more useful. More typically, we apply Fourier transforms (e.g., [5–7]) and/or Gaussian transforms (e.g., [8–10]) to effect these reductions.

A prior paper [11] introduced a fifth reduction method in the spirit of Fourier and Gaussian transforms that is an integral representation, having one fewer integral dimension than does a Gaussiantransform to represent a product of M Slater functions and roughly a quarter of the integral dimensions introduced by a Fourier transform for such a product. This is an advantage since the main drawback of using integral representations is that one adds to the number of integral dimensions one must ultimately solve. In each of these three methods, the reduction of those introduced integrals becomes more difficult the larger the numbers of wave functions transformed, so one fewer dimension is not a trivial advantage.

Gaussian transforms require a single one-dimensional integral for each wave function, and the completion of the square in the coordinate variables—to allow the angular integrals to be performed—can be undertaken in the resulting exponential. For Fourier transforms, on the other hand, one must introduce a three-dimensional integral for each wave function and often additional integrals to combine the resulting momentum denominators into a single denominator so that one can complete the square in the momenta [12]. Our prior work requires the introduction of one fewer integral dimension than does the Gaussian transform and many fewer than for Fourier transforms. Its main downside is that the resulting quadratic form (whose square one will complete) resides in a square root as the argument of a Macdonald function, for which there are fewer tabled integrals than for the exponential function wherein resides the quadratic form of Gaussian transforms.

The present paper derives four integral representations over finite intervals to represent a product of Slater orbitals. Often written as ψ_{000}, the Slater orbital $\frac{e^{-\eta x}}{x}$ acts as a seed function from which Slater functions [13], Hylleraas powers [7], and hydrogenic wave functions are derived by differentiation. (Known as the Yukawa [14] exchange potential in nuclear physics, this function also appears in plasma physics, where it is known as the Debye–Hückel potential, arising from screened charges [15] requiring the replacement of the Coulomb potential by an effective screened potential [16,17]. Such screening of charges also appears in solid-state physics, where this function is called the Thomas–Fermi potential. In the atomic physics of negative ions, the radial wave function is given by the equivalent Macdonald function $\left(R(r) = \frac{C}{\sqrt{r}} K_{1/2}(\eta r)\right)$ [18]. This function also appears in the approximate ground state wave function [19] for a hydrogen atom interacting with hypothesized non-zero-mass photons [20]. We will simply call these *Slater orbitals* herein.)

We start with the simplest integral requiring transformation, the product of two Slater orbitals integrated over all space,

$$S_1^{\eta_1 0 \eta_{12} 0}(0;0,\mathbf{x}_2) \equiv S_1^{\eta_1 j_1 \eta_{12} j_2}(\mathbf{p}_1;\mathbf{y}_1,\mathbf{y}_2)_{p_1\to 0, y_1, \to 0, y_2 \to x_2, j_1 \to 0, j_2 \to 0} = \int d^3x_1 \frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_{12} x_{12}}}{x_{12}} \quad , \tag{1}$$

where we use the much more general notation of the previous work [10] in which the short-hand form for shifted coordinates is $\mathbf{x}_{12} = \mathbf{x}_1 - \mathbf{x}_2$, $\mathbf{p}_1$ is a momentum variable within any plane wave associated with the (first) integration variable, the $\mathbf{y}_i$ are coordinates external to the integration, and the js are defined in the Gaussian transform [10] of the generalized Slater orbital:

$$\begin{aligned} V^{\eta j}(\mathbf{R}) &= R^{j-1} e^{-\eta R} = (-1)^j \frac{d^j}{d\eta^j} \frac{1}{\sqrt{\pi}} \int_0^\infty d\rho \frac{e^{-R^2 \rho} e^{-\eta^2/(4\rho)}}{\rho^{1/2}} \quad [\eta \geqq 0,\ R > 0] \quad . \\ &= \frac{1}{2^j \sqrt{\pi}} \int_0^\infty d\rho \frac{e^{-R^2\rho} e^{-\eta^2/(4\rho)}}{\rho^{(j+1)/2}} H_j\left(\frac{\eta}{2\sqrt{\rho}}\right) \quad [\forall j \geq 0 \text{ if } \eta > 0,\ j = 0 \text{ if } \eta = 0] \end{aligned} \tag{2}$$

In our prior work, we showed how Gaussian transforms can reduce this integral in roughly eight steps, so this time we will use Fourier transforms [21] (p. 512 No. 3.893.1, p. 382 No. 3.461.2, p. 384 No. 3.471.9):

$$
\begin{aligned}
S_1^{\eta_1 0 \eta_2 0}(0;0,x_2) = & \int d^3x_1 \frac{e^{-\eta_1 x_1}}{x_1}\frac{e^{-\eta_{12} x_{12}}}{x_{12}} \\
= & \int d^3x_1 \frac{1}{2\pi^2}\int d^3k_1 \frac{e^{i\,\mathbf{k}_1\cdot\mathbf{x}_1}}{(\eta_1^2+k_1^2)}\frac{1}{2\pi^2}\int d^3k_2 \frac{e^{i\,\mathbf{k}_2\cdot(\mathbf{x}_1-\mathbf{x}_2)}}{(\eta_{12}^2+k_2^2)} \\
= & \frac{2}{\pi}\int d^3k_1 \frac{1}{(\eta_1^2+k_1^2)}\int d^3k_2 \frac{e^{-i\,\mathbf{k}_2\cdot\mathbf{x}_2}}{(\eta_{12}^2+k_2^2)}\delta(\mathbf{k}_1+\mathbf{k}_2) \\
= & \frac{2}{\pi}\int d^3k_2 \frac{1}{(\eta_1^2+k_2^2)}\frac{e^{-i\,\mathbf{k}_2\cdot\mathbf{x}_2}}{(\eta_{12}^2+k_2^2)} \\
= & \frac{2}{\pi}\int d^3k_2 \int_0^1 d\alpha_1 \frac{1}{\left(\alpha_1(k_2^2+\eta_1^2)+(1-\alpha_1)(k_2^2+\eta_{12}^2)\right)^2} e^{-i\,\mathbf{k}_2\cdot\mathbf{x}_2} \\
= & \frac{2}{\pi}\int d^3k_2 \int_0^1 d\alpha_1 \int_0^\infty d\rho\rho \\
\times & \exp\Big(-i\,\mathbf{k}_2\cdot\mathbf{x}_2 - \rho\Big(\alpha_1\Big(k_2^2+\eta_1^2\Big)+(1-\alpha_1)\Big(k_2^2+\eta_{12}^2\Big)\Big)\Big) \\
= & \frac{2}{\pi}\int d^3k_2' \int_0^1 d\alpha_1 \int_0^\infty d\rho\rho \exp\left(-\rho k_2'^2 - \frac{x_2^2}{4\rho} - \rho\Big(\alpha_1\Big(\eta_1^2-\eta_{12}^2\Big)+\eta_{12}^2\Big)\right) \\
= & \frac{2}{\pi}4\pi \int_0^1 d\alpha_1 \int_0^\infty d\rho\rho \frac{\sqrt{\pi}}{4\rho^{3/2}} \exp\left(-\frac{x_2^2}{4\rho} - \rho\Big(\alpha_1\Big(\eta_1^2-\eta_{12}^2\Big)+\eta_{12}^2\Big)\right) \\
= & 2\pi \int_0^1 d\alpha_1 \frac{e^{-x_2\sqrt{\alpha_1(\eta_1^2-\eta_{12}^2)+\eta_{12}^2}}}{\sqrt{\alpha_1(\eta_1^2-\eta_{12}^2)+\eta_{12}^2}} \\
= & \frac{(4\pi)}{x_2(\eta_1^2-\eta_{12}^2)}\int_{x_2\eta_{12}}^{x_2\eta_1} e^{-y}\,dy \\
= & \frac{4\pi(e^{-\eta_{12}x_2}-e^{-\eta_1 x_2})}{x_2(\eta_1^2-\eta_{12}^2)} \quad .
\end{aligned} \tag{3}
$$

This is a considerably lengthy derivation, and the Gaussian transform approach is not much better. Of course, in this simple case, one can invoke the addition theorem expression for $e^{-i\,\mathbf{k}_2\cdot\mathbf{x}_2}$ in the fourth line to shorten the reduction, but for the large-M equivalent, the above process is what one must follow. (Actually, one would do well to avoid the use of the Dirac delta function in the third line when dealing with large M.)

The length of such derivations was the motivation for the fifth path to a solution given in our prior paper and for the present approach.

2. A Simpler Integral Representation

We begin by introducing an integral representation over a finite interval for a pair product of Slater orbitals,

$$
\frac{e^{-\eta_1 x_1}}{x_1}\frac{e^{-\eta_{12} x_{12}}}{x_{12}} = \int_0^1 d\alpha_1 \frac{\sqrt{(1-\alpha_1)\eta_1^2+\alpha_1\eta_{12}^2}\,K_1\left(\sqrt{\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1}}\sqrt{(1-\alpha_1)\eta_1^2+\alpha_1\eta_{12}^2}\right)}{\pi(1-\alpha_1)^{3/2}\alpha_1^{3/2}\sqrt{\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1}}} \quad , \tag{4}
$$

whose derivation will follow a display of its utility. We insert it as a replacement for the second line in the above problem, complete the square in the quadratic form, and then change variables from $\mathbf{x}_1$ to $\mathbf{x}_1' = \mathbf{x}_1 - (1-\alpha_1)\mathbf{x}_2$ (with unit Jacobian) in both places in the integrand where it appears. This gives [21] (p. 727. No. 6.596.3; p. 111 No. 2.311)

$$\begin{aligned}
S_1^{\eta_1 0 \eta_{12} 0}(0;0,x_2) &= \int d^3x_1 \int_0^1 d\alpha_1 \frac{\sqrt{(1-\alpha_1)\eta_1^2 + \alpha_1\eta_{12}^2}.}{\pi(1-\alpha_1)^{3/2}\alpha_1^{3/2}\sqrt{\frac{x_1^2}{1-\alpha_1} + \frac{x_{12}^2}{\alpha_1}}} \\
&\times K_1\left(\sqrt{\frac{x_1^2}{1-\alpha_1} + \frac{x_{12}^2}{\alpha_1}}\sqrt{(1-\alpha_1)\eta_1^2 + \alpha_1\eta_{12}^2}\right) \\
&= \int d^3x_1' \int_0^1 d\alpha_1 \frac{\sqrt{(1-\alpha_1)\eta_1^2 + \alpha_1\eta_{12}^2}}{\pi(1-\alpha_1)^{3/2}\alpha_1^{3/2}\sqrt{\frac{x_1'^2}{(1-\alpha_1)\alpha_1} + x_2^2}} \\
&\times K_1\left(\sqrt{\frac{x_1'^2}{(1-\alpha_1)\alpha_1} + x_2^2}\sqrt{(1-\alpha_1)\eta_1^2 + \alpha_1\eta_{12}^2}\right) \\
&= \int_0^1 d\alpha_1 \frac{2\pi e^{-x_2\sqrt{(1-\alpha_1)\eta_1^2+\alpha_1\eta_{12}^2}}}{\sqrt{(1-\alpha_1)\eta_1^2 + \alpha_1\eta_{12}^2}} = \int_{x_2\eta_1}^{x_2\eta_{12}} dy \frac{4\pi e^{-y}}{x_2(\eta_{12}^2 - \eta_1^2)} \\
&= \frac{4\pi(e^{-\eta_{12}x_2} - e^{-\eta_1 x_2})}{x_2(\eta_1^2 - \eta_{12}^2)} \quad ,
\end{aligned} \tag{5}$$

which is indeed a much shorter path to the solution than the Fourier and Gaussian transforms give. This follows from the fact that it requires the introduction of one integral to represent a pair product of Slater orbitals rather than one integral for *each* orbital that the Gaussian transform requires or the three-dimensional integral that the Fourier transform approach requires for each Slater orbital (with two additional integrals required, as in (4)).

Note that this new integral representation has a similar integrand to the integral representation introduced in our prior paper for products of M Slater orbitals,

$$\begin{aligned}
\frac{e^{-R_1\eta_1}}{R_1}\frac{e^{-R_2\eta_2}}{R_2}\cdots\frac{e^{-R_M\eta_M}}{R_M} &= \frac{1}{2^M\pi^{2M}}\int_0^\infty d\zeta_1\int_0^\infty d\zeta_2\cdots\int_0^\infty d\zeta_{M-1}\frac{\pi^{3M/2}}{\prod_{i=1}^{M-1}\zeta_i^{3/2}}2^{\frac{M}{2}+1} \\
&\times \left(R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \cdots + \frac{R_M^2}{\zeta_{M-1}}\right)^{-M/4}\left(\eta_1^2 + \zeta_1\eta_2^2 + \zeta_2\eta_3^2 + \cdots + \zeta_{M-1}\eta_M^2\right)^{M/4} \\
&\times K_{\frac{M}{2}}\left(\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \cdots + \frac{R_M^2}{\zeta_{M-1}}}\sqrt{\eta_1^2 + \zeta_1\eta_2^2 + \zeta_2\eta_3^2 + \cdots + \zeta_{M-1}\eta_M^2}\right) \quad ,
\end{aligned} \tag{6}$$

except that the new integral representation has finite limits of integration rather than the infinite intervals of the previous work.

3. A Derivation Sketch

The first step in creating the prior integral representation—and the new one—entails converting a product of Slater orbitals into denominators of some power (combined with other factors) using some *initial* integral representation, such as via the Stieltjes transform [22] or [21] (p.706 No. 6.554.4); in the following, we use [21] (p. 467 No. 3.773.5):

$$\frac{e^{-\eta_1 x_1}}{x_1}\frac{e^{-\eta_{12}x_{12}}}{x_{12}} = \int_0^\infty\int_0^\infty dt_1 dt_2 \frac{2}{\pi}\frac{\cos(t_1\eta_1)}{(t_1^2 + x_1^2)}\frac{2}{\pi}\frac{\cos(t_2\eta_{12})}{(t_2^2 + x_{12}^2)} \quad . \tag{7}$$

In the prior paper, we combined products of denominators into one, consolidating the coordinate variables into a common quadratic form, using [21] (p. 649 No. 4.638.2)

$$\frac{1}{r_1^{p_1} r_2^{p_2} \cdots r_n^{p_n} r_0^{s-p_1-p_2-\cdots-p_n}} = \frac{\Gamma(s)}{\Gamma(s-p_1-p_2-\cdots-p_n)\Gamma(p_1)\Gamma(p_2)\cdots\Gamma(p_n)}$$
$$\times \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \cdots \int_0^\infty d\zeta_n \frac{\zeta_1^{p_1-1}\zeta_1^{p_2-1}\cdots\zeta_1^{p_n-1}}{(r_0+r_1\zeta_1+r_2\zeta_2+\cdots+r_n\zeta_n)^s}$$
$$[p_i > 0,\, r_i > 0,\, s > p_1+p_2+\cdots+p_n > 0] \quad , \tag{8}$$

(with $p_1 = 1$ and $s = 2$ for $n = 1$):

$$\frac{e^{-\eta_1 x_1}}{x_1}\frac{e^{-\eta_{12} x_{12}}}{x_{12}} = \frac{4}{\pi^2}\int_0^\infty\int_0^\infty dt_1 dt_2 \cos(t_1\eta_1)\cos(t_2\eta_{12})\int_0^\infty d\zeta_1 \frac{\zeta_1^{1-1}}{\left(\zeta_1(t_1^2+x_1^2)+(t_2^2+x_{12}^2)\right)^2} . \tag{9}$$

One then performs the t integrals to obtain the $n = 2$ version of (6).

While conceptually easy to follow, the subsequent integration of the ts as M increases beyond 3 produces functions whose arguments do not form discernible patterns, so we were not able to generalize this approach (using [21] (p. 467 No. 3.773.5)) to large M in either the prior or the present paper.

4. Full Derivation of a Finite-Interval Integral Representation for M Slater Orbitals

To represent a product of M Slater orbitals using finite-interval integrals, one can in principle use Feynman parametrization [23] as extended by Schweber in three formulations [24]. Schweber's first parametrization gives an M-dimensional integral with an embedded Dirac delta function that will ultimately remove one integral. We found this form less easy to work with than the other two.

Schweber's second parametrization,

$$\frac{1}{D_1 D_2 \cdots D_n} = (n-1)! \int_0^1 d\alpha_1 \int_0^{\alpha_1} d\alpha_2 \cdots \int_0^{\alpha_{n-2}} d\alpha_{n-1}$$
$$\times \frac{1}{(D_n\alpha_{n-1} + D_{n-1}(\alpha_{n-2}-\alpha_{n-1}) + \cdots + D_1(1-\alpha_1))^n} \tag{10}$$

looks somewhat dubious for analytical uses since each succeeding integral has the prior parameter as its upper limit. It turns out, however, that one can perform a change of variables in each integral at the end of the derivation to give all integrals over [0, 1].

In our prior work, we used Fourier transforms to convert the product of M Slater orbitals into denominators instead of the integral set using [21] (p. 467 No. 3.773.5), which we utilized in Equation (7). Since Fourier transforms include momentum variables in plane waves, we take the additional step of moving the combined momentum denominator into an exponential by using [21] (p. 364 No. 3.381.4).

$$(\nu-1)!D^{-\nu} = \int_0^\infty d\rho\rho^{\nu-1}e^{-\rho D} \quad . \tag{11}$$

Thus, for a product of M Slater orbitals, we have [21] (p. 649 No. 4.638.2).

$$
\begin{aligned}
\frac{e^{-R_1\eta_1}}{R_1}\,\frac{e^{-R_2\eta_2}}{R_2}\cdots\frac{e^{-R_M\eta_M}}{R_M} &= \int d^3k_1 \int d^3k_2 \cdots \int d^3k_M \\
&\times \quad \frac{1}{2\pi^2}\cdot\frac{e^{ik_1\cdot R_1}}{k_1^2+\eta_1^2}\cdot\frac{1}{2\pi^2}\cdot\frac{e^{ik_2\cdot R_2}}{k_2^2+\eta_2^2}\cdots\frac{1}{2\pi^2}\cdot\frac{e^{ik_M\cdot R_M}}{k_M^2+\eta_M^2} \\
&= \int_0^1 d\alpha_1 \int_0^{\alpha_1} d\alpha_2 \cdots \int_0^{\alpha_{M-2}} d\alpha_{M-1} \int d^3k_1 \int d^3k_2 \cdots \int d^3k_M \frac{(M-1)!}{2^M\pi^{2M}} \\
&\times \quad \exp(ik_1\cdot R_1 + ik_2\cdot R_2 + \cdots + ik_{M-1}\cdot x_{M-1} + ik_M\cdot R_M) \\
&\times \Big[\Big(k_1^2+\eta_1^2\Big)(1-\alpha_1) + \Big(k_2^2+\eta_2^2\Big)(\alpha_1-\alpha_2) + \cdots \\
&\qquad \cdots + \Big(k_{M-1}^2+\eta_{M-1}^2\Big)(\alpha_{M-2}-\alpha_{M-1}) + \Big(k_M^2+\eta_M^2\Big)\alpha_M\Big]^{-M} \\
&= \frac{1}{2^M\pi^{2M}} \int_0^\infty d\rho \int_0^1 d\alpha_1 \int_0^{\alpha_1} d\alpha_2 \cdots \int_0^{\alpha_{M-2}} d\alpha_{M-1} \int d^3k_1 \int d^3k_2 \cdots \int d^3k_M \rho^{M-1} \\
&\times \exp(-\rho(ik_1\cdot R_1/\rho + ik_2\cdot R_2/\rho + \cdots + ik_{M-1}\cdot x_{M-1}/\rho + ik_M\cdot R_M/\rho)) \\
&\times \quad exp\Big[-\rho\Big(\Big(k_1^2+\eta_1^2\Big)(1-\alpha_1) + \Big(k_2^2+\eta_2^2\Big)(\alpha_1-\alpha_2) + \cdots \\
&+ \cdots + \Big(k_{M-1}^2+\eta_{M-1}^2\Big)(\alpha_{M-2}-\alpha_{M-1}) + \Big(k_M^2+\eta_M^2\Big)\alpha_M\Big)\Big] \\
&\equiv \frac{1}{2^M\pi^{2M}} \int_0^\infty d\rho \int_0^1 d\alpha_1 \int_0^{\alpha_1} d\alpha_2 \cdots \int_0^{\alpha_{M-2}} d\alpha_{M-1} \int d^3k_1 \int d^3k_2 \cdots \int d^3k_M \\
&\times \quad \rho^{M-1}\exp(-\rho\, Q) \quad .
\end{aligned} \tag{12}
$$

The quadratic form can be written as [12]

$$Q = \underline{V}^T \underline{W}\,\underline{V} \quad , \tag{13}$$

where

$$\underline{V}^T = (\mathbf{k}_1, \mathbf{k}_2, \cdots, \mathbf{k}_M, 1) \quad , \tag{14}$$

$$\underline{W} = \begin{pmatrix} (1-\alpha_1) & 0 & \cdots & 0 & 0 & \mathbf{b}_1 \\ 0 & (\alpha_1-\alpha_2) & \cdots & 0 & 0 & \mathbf{b}_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & (\alpha_{M-2}-\alpha_{M-1}) & 0 & \mathbf{b}_{M-1} \\ 0 & 0 & \cdots & 0 & \alpha_{M-1} & \mathbf{b}_M \\ \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_{M-1} & \mathbf{b}_M & C \end{pmatrix} , \tag{15}$$

$$C = (1-\alpha_1)\eta_1^2 + (\alpha_1-\alpha_2)\eta_2^2 + \cdots + (\alpha_{M-2}-\alpha_{M-1})\eta_{M-1}^2 + \alpha_{M-1}\eta_M^2 \quad , \tag{16}$$

and

$$\mathbf{b_j} = -\frac{i}{2\rho}\mathbf{R_j} \quad . \tag{17}$$

Now suppose one could find an orthogonal transformation that reduced Q to diagonal form

$$Q' = a_1' k_1'^2 + a_2' k_2'^2 + \ldots + a_{N+M}' k_{N+M}'^2 + c', \tag{18}$$

where, as shown by Chisholm [25], the a' are positive. Then, after a simple translation in $\{\mathbf{k}_1, \mathbf{k}_2, \cdots, \mathbf{k}_M\}$ space (with Jacobian = 1), the k integrals could be performed [21] (p. 382 No. 3.461.2),

$$\int d^3k_1' \ldots d^3k_M' e^{-\rho\left(a_1' k_1'^2 + a_2' k_2'^2 + \ldots + a_M' k_M'^2\right)} = \left(\frac{\pi^M}{\rho^M \Lambda}\right)^{3/2} . \tag{19}$$

Since this result is expressed in the form of an invariant determinant,

$$\Lambda = \begin{vmatrix} (1-\alpha_1) & 0 & \cdots & 0 & 0 \\ 0 & (\alpha_1-\alpha_2) & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & (\alpha_{M-2}-\alpha_{M-1}) & 0 \\ 0 & 0 & \cdots & 0 & \alpha_{M-1} \end{vmatrix} , \tag{20}$$
$$= (1-\alpha_1)\left(\prod_{i=2}^{M-1}(\alpha_{i-1}-\alpha_i)\right)\alpha_{M-1} = \prod_{i=1}^{M} a_i'$$

actually finding the orthogonal transformation that reduces Q to diagonal form is unnecessary. What is left to find is just the exponential of $-\rho c'$, which we integrate over ρ and the α_i.

This orthogonal transformation also leaves

$$\Omega = \det \underline{W} \tag{21}$$

invariant, and to find its value, one need only expand Ω by minors:

$$\begin{aligned} \Omega &= C\Lambda + \sum_{i=1}^{M}\sum_{j=1}^{M} \mathbf{b}_i \cdot \mathbf{b}_j (-1)^{i+j+1}\Lambda_{ij} \\ &= C\Lambda - b_1^2\left(\prod_{i=2}^{M-1}(\alpha_{i-1}-\alpha_i)\right)\alpha_{M-1} - \sum_{j=2}^{M-1} b_j^2 \frac{(1-\alpha_1)}{\alpha_{j-1}-\alpha_j}\left(\prod_{i=2}^{M-1}(\alpha_{i-1}-\alpha_i)\right)\alpha_{M-1} \\ &- b_M^2(1-\alpha_1)\prod_{i=2}^{M-1}(\alpha_{i-1}-\alpha_i) \quad , \end{aligned} \tag{22}$$

where Λ_{ij} is Λ with the ith row and jth column deleted and is diagonal in the present case. Therefore, c' (of (18)) is given by

$$\begin{aligned} c' = \Omega/\Lambda &= (1-\alpha_1)\eta_1^2 + \sum_{j=2}^{M-1}\eta_j^2(\alpha_{j-1}-\alpha_j) + \alpha_{M-1}\eta_M^2 - \frac{b_1^2}{(1-\alpha_1)} - \sum_{j=2}^{M-1}\frac{b_j^2}{(\alpha_{j-1}-\alpha_j)} \\ &- \frac{b_M^2}{\alpha_{M-1}} \\ &= (1-\alpha_1)\eta_1^2 + \sum_{j=2}^{M-1}\eta_j^2(\alpha_{j-1}-\alpha_j) + \alpha_{M-1}\eta_M^2 + \frac{1}{4\rho^2}\frac{R_1^2}{(1-\alpha_1)} \\ &+ \sum_{j=2}^{M-1}\frac{1}{4\rho^2}\frac{R_j^2}{(\alpha_{j-1}-\alpha_j)} + \frac{1}{4\rho^2}\frac{b_M^2}{\alpha_{M-1}} \quad , \end{aligned} \tag{23}$$

so that

$$\begin{aligned} \frac{e^{-R_1\eta_1}}{R_1}\frac{e^{-R_2\eta_2}}{R_2}\cdots\frac{e^{-R_M\eta_M}}{R_M} &= \frac{1}{2^M\pi^{2M}}\int_0^\infty d\rho \int_0^1 d\alpha_1 \int_0^{\alpha_1} d\alpha_2 \cdots \int_0^{\alpha_{M-2}} d\alpha_{M-1} \\ \times & \frac{\pi^{3M/2}}{\rho^{M/2+1}\left((1-\alpha_1)\left(\prod_{i=2}^{M-1}(\alpha_{i-1}-\alpha_i)\right)\alpha_{M-1}\right)^{3/2}} \\ \times & \, exp\left[-\rho\left((1-\alpha_1)\eta_1^2 + (\alpha_1-\alpha_2)\eta_2^2 + \cdots + (\alpha_{M-2}-\alpha_{M-1})\eta_{M-1}^2 + \cdots + \alpha_{M-1}\eta_M^2\right)\right] \\ \times & \, exp\left(-\left(\frac{R_1^2}{(1-\alpha_1)} + \frac{R_2^2}{(\alpha_1-\alpha_2)} + \cdots + \frac{R_{M-1}^2}{(\alpha_{M-2}-\alpha_{M-1})} + \frac{R_M^2}{\alpha_{M-1}}\right)\frac{1}{4\rho}\right) \quad . \end{aligned} \tag{24}$$

We perform the ρ integral [21] (p. 384 No. 3.471.9) to give the most compact, semifinal form for the desired integral representation:

$$\begin{aligned} \frac{e^{-R_1\eta_1}}{R_1}\frac{e^{-R_2\eta_2}}{R_2}\cdots\frac{e^{-R_M\eta_M}}{R_M} &= \int_0^1 d\alpha_1\int_0^{\alpha_1} d\alpha_2\cdots\int_0^{\alpha_{M-2}} d\alpha_{M-1} \\ &\times \quad \frac{2^{1-\frac{M}{2}}\pi^{-M/2}}{(1-\alpha_1)^{3/2}\left(\prod_{i=2}^{M-1}(\alpha_{i-1}-\alpha_i)^{3/2}\right)\alpha_{M-1}^{3/2}} \\ &\times \quad \left((1-\alpha_1)\eta_1^2+(\alpha_1-\alpha_2)\eta_2^2+\cdots+(\alpha_{M-2}-\alpha_{M-1})\eta_{M-1}^2+\cdots+\alpha_{M-1}\eta_M^2\right)^{M/4} \\ &\times \quad \left(\frac{R_1^2}{(1-\alpha_1)}+\frac{R_2^2}{(\alpha_1-\alpha_2)}+\cdots+\frac{R_{M-1}^2}{(\alpha_{M-2}-\alpha_{M-1})}+\frac{R_M^2}{\alpha_{M-1}}\right)^{-M/4} \\ &\times \quad K_{\frac{M}{2}}\left(\sqrt{(1-\alpha_1)\eta_1^2+(\alpha_1-\alpha_2)\eta_2^2+\cdots+(\alpha_{M-2}-\alpha_{M-1})\eta_{M-1}^2+\cdots+\alpha_{M-1}\eta_M^2}\right. \\ &\times \quad \left.\sqrt{\frac{R_1^2}{(1-\alpha_1)}+\frac{R_2^2}{(\alpha_1-\alpha_2)}+\cdots+\frac{R_{M-1}^2}{(\alpha_{M-2}-\alpha_{M-1})}+\frac{R_M^2}{\alpha_{M-1}}}\right) \quad . \end{aligned} \tag{25}$$

5. Unifying the Upper Limits of the Integrals to Give a Second Integral Representation

The above forms are fine for numerical integration, but for $M > 2$, their utility is somewhat hampered for analytical reduction since each succeeding integral has the prior parameter as its upper limit. One can cast each such integral into one over the interval $[0, 1]$ by making a change of variables to

$$\alpha_j \rightarrow \alpha_{j-1}\sigma_j \tag{26}$$

in sequence from $j = M-1$ down to $j = 2$ and multiplying by the Jacobian that consists of the product of derivatives of α_j/α_{j-1} that defines each new variable σ_j,

$$\prod_{j=1}^{M-2}\frac{1}{\alpha_j} \quad . \tag{27}$$

The first three such are, where we explicitly put in the shifted coordinates $R_j^2 = x_{1j}^2$ (and corresponding parameters $\eta_j^2 = \eta_{1j}^2$),

$$\begin{aligned} \frac{e^{-x_1\eta_1}}{x_1}\frac{e^{-x_{12}\eta_{12}}}{x_{12}}\frac{e^{-x_{13}\eta_{13}}}{x_{13}} &= \int_0^1 d\alpha_1\int_0^1 d\sigma_2\frac{\alpha_1\left((1-\alpha_1)\eta_1^2+\alpha_1(1-\sigma_2)\eta_{12}^2+\alpha_1\sigma_2\eta_{13}^2\right)^{3/4}}{\sqrt{2}\pi^{3/2}\left((1-\alpha_1)\alpha_1^2(1-\sigma_2)\sigma_2\right)^{3/2}} \\ &\times \quad \left(\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1(1-\sigma_2)}+\frac{x_{13}^2}{\alpha_1\sigma_2}\right)^{-3/4} \\ &\times \quad K_{\frac{3}{2}}\left(\sqrt{\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1(1-\sigma_2)}+\frac{x_{13}^2}{\alpha_1\sigma_2}}\sqrt{(1-\alpha_1)\eta_1^2+\alpha_1(1-\sigma_2)\eta_{12}^2+\alpha_1\sigma_2\eta_{13}^2}\right) \quad , \end{aligned} \tag{28}$$

$$\begin{aligned} \frac{e^{-x_1\eta_1}}{x_1}\frac{e^{-x_{12}\eta_{12}}}{x_{12}}\frac{e^{-x_{13}\eta_{13}}}{x_{13}}\frac{e^{-x_{14}\eta_{14}}}{x_{14}} &= \int_0^1 d\alpha_1\int_0^1 d\sigma_2\int_0^1 d\sigma_3 \\ &\times \quad \frac{\alpha_1^2\sigma_2\left((1-\alpha_1)\eta_1^2+\eta_{12}^2\alpha_1(1-\sigma_2)+\eta_{13}^2\alpha_1\sigma_2(1-\sigma_3)+\eta_{14}^2\alpha_1\sigma_2\sigma_3\right)}{2\pi^2\left((1-\alpha_1)\alpha_1^3(1-\sigma_2)\sigma_2^2(1-\sigma_3)\sigma_3\right)^{3/2}} \\ &\times \quad \left(\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1(1-\sigma_2)}+\frac{x_{13}^2}{\alpha_1\sigma_2(1-\sigma_3)}+\frac{x_{14}^2}{\alpha_1\sigma_2\sigma_3}\right)^{-1} \\ &\times \quad K_2\left[\sqrt{\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1(1-\sigma_2)}+\frac{x_{13}^2}{\alpha_1\sigma_2(1-\sigma_3)}+\frac{x_{14}^2}{\alpha_1\sigma_2\sigma_3}}\right. \\ &\times \quad \left.\sqrt{(1-\alpha_1)\eta_1^2+\eta_{12}^2\alpha_1(1-\sigma_2)+\eta_{13}^2\alpha_1\sigma_2(1-\sigma_3)+\eta_{14}^2\alpha_1\sigma_2\sigma_3}\right] \quad , \end{aligned} \tag{29}$$

and

$$
\begin{aligned}
\frac{e^{-x_1\eta_1}}{x_1}\frac{e^{-x_{12}\eta_{12}}}{x_{12}}\frac{e^{-x_{13}\eta_{13}}}{x_{13}}\frac{e^{-x_{14}\eta_{14}}}{x_{14}}\frac{e^{-x_{15}\eta_{15}}}{x_{15}} &= \int_0^1 d\alpha_1 \int_0^1 d\sigma_2 \int_0^1 d\sigma_3 \int_0^1 d\sigma_4 \\
\times &\quad \frac{\alpha_1^3\sigma_2^2\sigma_3\left(\sqrt{(1-\alpha_1)\eta_1^2+\eta_{12}^2\alpha_1(1-\sigma_2)+\eta_{13}^2\alpha_1\sigma_2(1-\sigma_3)+\eta_{14}^2\alpha_1\sigma_2\sigma_3(1-\sigma_4)+\eta_{15}^2\alpha_1\sigma_2\sigma_3\sigma_4}\right)^{5/4}}{2\sqrt{2}\pi^{5/2}\left((1-\alpha_1)\alpha_1^4(1-\sigma_2)\sigma_2^3(1-\sigma_3)\sigma_3^2(1-\sigma_4)\sigma_4\right)^{3/2}} \\
\times &\quad \left(\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1(1-\sigma_2)}+\frac{x_{13}^2}{\alpha_1\sigma_2(1-\sigma_3)}+\frac{x_{14}^2}{\alpha_1\sigma_2\sigma_3(1-\sigma_4)}+\frac{x_{15}^2}{\alpha_1\sigma_2\sigma_3\sigma_4}\right)^{-5/4} \\
\times &\quad K_{\frac{5}{2}}\left[\sqrt{\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1(1-\sigma_2)}+\frac{x_{13}^2}{\alpha_1\sigma_2(1-\sigma_3)}+\frac{x_{14}^2}{\alpha_1\sigma_2\sigma_3(1-\sigma_4)}+\frac{x_{15}^2}{\alpha_1\sigma_2\sigma_3\sigma_4}}\right. \\
\times &\quad \left.\sqrt{(1-\alpha_1)\eta_1^2+\eta_{12}^2\alpha_1(1-\sigma_2)+\eta_{13}^2\alpha_1\sigma_2(1-\sigma_3)+\eta_{14}^2\alpha_1\sigma_2\sigma_3(1-\sigma_4)+\eta_{15}^2\alpha_1\sigma_2\sigma_3\sigma_4}\right] .
\end{aligned}
\tag{30}
$$

This can easily be seen to generalize to

$$
\begin{aligned}
\frac{e^{-R_1\eta_1}}{R_1}\frac{e^{-R_2\eta_2}}{R_2}\cdots\frac{e^{-R_M\eta_M}}{R_M} &= \int_0^1 d\alpha_1 \int_0^1 d\sigma_2 \int_0^1 d\sigma_3 \cdots \int_0^1 d\sigma_{M-1} \\
&\times \frac{2^{-(M-2)/2}\pi^{-M/2}\alpha_1^{M-2}\sigma_2^{M-3}\sigma_3^{M-4}\cdots\sigma_{M-2}}{\left((1-\alpha_1)\alpha_1^{M-1}(1-\sigma_2)\sigma_2^{M-2}(1-\sigma_3)\cdots\sigma_{M-2}^2(1-\sigma_{M-1})\sigma_{M-1}\right)^{3/2}} \\
&\times \big((1-\alpha_1)\eta_1^2+\eta_2^2\alpha_1(1-\sigma_2)+\eta_3^2\alpha_1\sigma_2(1-\sigma_3)+\cdots \\
&\qquad \cdots+\eta_{M-1}^2\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-2}(1-\sigma_{M-1})+\eta_M^2\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-1}\big)^{M/4} \\
&\times\left(\frac{R_1^2}{(1-\alpha_1)}+\frac{R_2^2}{\alpha_1(1-\sigma_2)}+\frac{R_3^2}{\alpha_1\sigma_2(1-\sigma_3)}+\cdots+\frac{R_{M-1}^2}{\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-2}(1-\sigma_{M-1})}+\frac{R_M^2}{\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-1}}\right)^{-M/4} \\
&\times K_{\frac{M}{2}}\Big(\big[(1-\alpha_1)\eta_1^2+\eta_2^2\alpha_1(1-\sigma_2)+\eta_3^2\alpha_1\sigma_2(1-\sigma_3)+\cdots \\
&\qquad \cdots+\eta_{M-1}^2\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-2}(1-\sigma_{M-1})+\eta_M^2\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-1}\big]^{1/2} \\
&\times\sqrt{\frac{R_1^2}{(1-\alpha_1)}+\frac{R_2^2}{\alpha_1(1-\sigma_2)}+\frac{R_3^2}{\alpha_1\sigma_2(1-\sigma_3)}+\cdots+\frac{R_{M-1}^2}{\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-2}(1-\sigma_{M-1})}+\frac{R_M^2}{\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-1}}}\Big) .
\end{aligned}
\tag{31}
$$

Inspection shows that for $M = 2$, we indeed obtain Equation (4).

One unusual feature of this integral representation is that, like that derived in the prior paper, the recursion relationships of Macdonald functions can be applied to lower (or raise) the indices.

Inclusion of Plane Waves and Dipole Interactions

Transition amplitudes sometimes contain plane waves, and these can be easily included in this integral representation directly in the ρ version,

$$
\begin{aligned}
\frac{e^{-R_1\eta_1}}{R_1}\frac{e^{-R_2\eta_2}}{R_2}\cdots\frac{e^{-R_M\eta_M}}{R_M} &= \int_0^\infty d\rho \int_0^1 d\alpha_1 \int_0^1 d\sigma_2 \int_0^1 d\sigma_3 \cdots \int_0^1 d\sigma_{M-1} \\
&\times \frac{2^{-M}\pi^{-M/2}\rho^{-(M+2)/2}\alpha_1^{M-2}\sigma_2^{M-3}\sigma_3^{M-4}\cdots\sigma_{M-2}}{\left((1-\alpha_1)\alpha_1^{M-1}(1-\sigma_2)\sigma_2^{M-2}(1-\sigma_3)\cdots\sigma_{M-2}^2(1-\sigma_{M-1})\sigma_{M-1}\right)^{3/2}} \\
&\times\ exp\big(-\rho\big((1-\alpha_1)\eta_1^2+\eta_2^2\alpha_1(1-\sigma_2)+\eta_3^2\alpha_1\sigma_2(1-\sigma_3)+\cdots \\
&\qquad \cdots+\eta_{M-1}^2\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-2}(1-\sigma_{M-1})+\eta_M^2\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-1}\big)\big) \\
&\times\ exp\Bigg(-\bigg(\frac{R_1^2}{(1-\alpha_1)}+\frac{R_2^2}{\alpha_1(1-\sigma_2)}+\frac{R_3^2}{\alpha_1\sigma_2(1-\sigma_3)}+\cdots \\
&\qquad \cdots+\frac{R_{M-1}^2}{\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-2}(1-\sigma_{M-1})}+\frac{R_M^2}{\alpha_1\sigma_2\sigma_3\cdots\sigma_{M-1}}\bigg)\frac{1}{4\rho}\Bigg)
\end{aligned}
\tag{32}
$$

prior to completing the square by utilizing an orthogonal transformation (like that for the k_j) that reduces the spatial-coordinate quadratic form to become diagonal. Again, one has invariant determinants for this orthogonal transformation so that it never needs to actually be explicitly found. As before, this is followed by a simple translation in $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\}$ space (with Jacobian = 1).

In the more compact version containing Macdonald functions, one can simply apply the translation in $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\}$ space to the plane wave(s) that multiply Equations (25), (31) and (37).

Photoionization transition amplitudes will generally contain dipole terms $\cos(\theta)$ that can be transformed into plane waves via a transformation like [26]

$$\cos\theta_{12} = -x_1^{-1}x_2^{-1}\frac{\partial}{\partial Q}e^{-Q\mathbf{x}_1\cdot\mathbf{x}_2}\Big|_{Q=0} \quad , \tag{33}$$

giving an integro-differential representation whose inclusion follows that for other sorts of plane waves.

6. A Third Integral Representation

Schweber's third parametrization, which can be derived by iterating [21] (p. 336 No. 3.199) and [27], is

$$\frac{1}{D_1}\frac{1}{D_2}\cdots\frac{1}{D_n} = (n-1)!\int_0^1 d\alpha_1\alpha_1^{n-2}\int_0^1 d\alpha_2\alpha_2^{n-3}\cdots\int_0^1 d\alpha_{n-1} \quad , \tag{34}$$
$$\times\frac{1}{(D_1\alpha_1\alpha_2\cdots\alpha_{n-1}+D_2\alpha_1\cdots\alpha_{n-2}(1-\alpha_{n-1})+\cdots+D_{n-1}\alpha_1(1-\alpha_2)+D_n(1-\alpha_1))^n}$$

so that, for instance,

$$\begin{aligned}\frac{e^{-\eta_1x_1}}{x_1}\frac{e^{-\eta_{12}x_{12}}}{x_{12}} &= \frac{4}{\pi^2}\int_0^\infty\int_0^\infty\cos(t_1\eta_1)\cos(t_2\eta_{12})dt_1dt_2\\ &\times\int_0^1 d\alpha_1\frac{1}{((t_1^2+x_1^2)\alpha_1+(t_2^2+x_{12}^2)(1-\alpha_1))^2}.\end{aligned} \tag{35}$$

However, to derive the integral representation for M products of Slater orbitals, we again utilize the Fourier transform approach, above, with Schweber's third parametrization of the resulting denominators, yielding

$$\begin{aligned}\frac{e^{-R_1\eta_1}}{R_1}\frac{e^{-R_2\eta_2}}{R_2}\cdots\frac{e^{-R_M\eta_M}}{R_M} &= \frac{1}{2^M\pi^{2M}}\int_0^\infty d\rho\int_0^1 d\alpha_1\int_0^1 d\alpha_2\cdots\int_0^1 d\alpha_{M-1}\\ &\times\alpha_1^{M-2}\alpha_2^{M-3}\cdots\alpha_{M-3}^2\alpha_{M-2}^1\\ &\times\frac{\pi^{3M/2}}{\rho^{M/2+1}\prod_{i=1}^{M-1}\alpha_i^{3(M-i)/2}(1-\alpha_i)^{3/2}}\\ &\times exp\Big(-\rho\Big(\alpha_1\alpha_2\cdots\alpha_{M-1}\eta_1^2+\alpha_1\alpha_2\cdots\alpha_{M-2}(1-\alpha_{M-1})\eta_2^2\\ &+\cdots+\alpha_1(1-\alpha_2)\eta_{M-1}^2+(1-\alpha_1)\eta_M^2\Big)\Big)\\ &\times exp\left(-\left(\frac{R_1^2}{\alpha_1\alpha_2\cdots\alpha_{M-1}}+\frac{R_2^2}{\alpha_1\alpha_2\cdots\alpha_{M-2}(1-\alpha_{M-1})}\right.\right.\\ &+\left.\left.\cdots+\frac{R_{M-1}^2}{\alpha_1(1-\alpha_2)}+\frac{R_M^2}{(1-\alpha_1)}\right)\frac{1}{4\rho}\right) \quad .\end{aligned} \tag{36}$$

We perform the ρ integral [21] (p. 384 No. 3.471.9) to give the most compact form,

$$\frac{e^{-R_1\eta_1}}{R_1}\frac{e^{-R_2\eta_2}}{R_2}\cdots\frac{e^{-R_M\eta_M}}{R_M} = \frac{1}{2^M\pi^{2M}}\int_0^1 d\alpha_1\int_0^1 d\alpha_2\cdots\int_0^1 d\alpha_{M-1}\alpha_1^{M-2}\alpha_2^{M-3}\cdots\alpha_{M-3}^2\alpha_{M-2}^1$$
$$\times \frac{\pi^{3M/2}2^{1+M/2}}{\prod_{i=1}^{M-1}\alpha_i^{3(M-i)/2}(1-\alpha_i)^{3/2}}\Big[\alpha_1\alpha_2\cdots\alpha_{M-1}\eta_1^2+\alpha_1\alpha_2\cdots\alpha_{M-2}(1-\alpha_{M-1})\eta_2^2+ \cdots+\alpha_1(1-\alpha_2)\eta_{M-1}^2+(1-\alpha_1)\eta_M^2\Big]^{M/4}$$
$$\times \left(\frac{R_1^2}{\alpha_1\alpha_2\cdots\alpha_{M-1}}+\frac{R_2^2}{\alpha_1\alpha_2\cdots\alpha_{M-2}(1-\alpha_{M-1})}+\cdots+\frac{R_{M-1}^2}{\alpha_1(1-\alpha_2)}+\frac{R_M^2}{(1-\alpha_1)}\right)^{-M/4} \quad (37)$$
$$\times K_{\frac{M}{2}}\Big[\big(\alpha_1\alpha_2\cdots\alpha_{M-1}\eta_1^2+\alpha_1\alpha_2\cdots\alpha_{M-2}(1-\alpha_{M-1})\eta_2^2+\cdots \cdots+\alpha_1(1-\alpha_2)\eta_{M-1}^2+(1-\alpha_1)\eta_M^2\big)^{1/2}$$
$$\times \sqrt{\frac{R_1^2}{\alpha_1\alpha_2\cdots\alpha_{M-1}}+\frac{R_2^2}{\alpha_1\alpha_2\cdots\alpha_{M-2}(1-\alpha_{M-1})}+\cdots+\frac{R_{M-1}^2}{\alpha_1(1-\alpha_2)}+\frac{R_M^2}{(1-\alpha_1)}}\Bigg],$$

The $M=3$ version is given explicitly as follows:

$$\frac{e^{-x_1\eta_1}}{x_1}\frac{e^{-x_{12}\eta_2}}{x_{12}}\frac{e^{-x_{13}\eta_{13}}}{x_{13}} = \int_0^1\int_0^1 d\alpha_1 d\alpha_2\frac{\alpha_1\left(\alpha_1\alpha_2\eta_1^2+\alpha_1(1-\alpha_2)\eta_{12}^2+(1-\alpha_1)\eta_{13}^2\right)^{3/4}}{\sqrt{2}\pi^{3/2}\left((1-\alpha_1)\alpha_1^2(1-\alpha_2)\alpha_2\right)^{3/2}}$$
$$\times \left(\frac{x_1^2}{\alpha_1\alpha_2}+\frac{x_{12}^2}{\alpha_1(1-\alpha_2)}+\frac{x_{13}^2}{1-\alpha_1}\right)^{-3/4} \quad (38)$$
$$\times K_{\frac{3}{2}}\left(\sqrt{\frac{x_1^2}{\alpha_1\alpha_2}+\frac{x_{12}^2}{\alpha_1(1-\alpha_2)}+\frac{x_{13}^2}{1-\alpha_1}}\sqrt{\alpha_1\alpha_2\eta_1^2+\alpha_1(1-\alpha_2)\eta_{12}^2+(1-\alpha_1)\eta_{13}^2}\right)$$

Comparison with (28) shows that the associations of the integration parameters with x_{13}^2 and x_1^2 have been reversed, as have their associations with η_{13}^2 and η_1^2. This may or may not be an advantage in subsequent integrations after completing the square in x_1 for $M \geq 3$.

7. Utilizing Meijer G-Functions to Reduce Integrals

The utility of these new integral transformations for large M may well hinge on finding integrals over variables that reside within square roots as the argument of a Macdonald function. One method for crafting such untabled integrals is to violate two general rules of procedure in the analytic reduction of integrals. The first rule is to use sequential integration whenever possible. For instance, if one adds a third unshifted Slater orbital to Equation (1) and integrates over both variables, one would reasonably start by transforming only those Slater orbitals that contain x_1 and integrate over that variable. Next, one integrates the resultant and the third Slater orbital over x_2. The result is easily found to be [21] (p. 358 No. 3.351.3)

$$\begin{aligned} S_1^{\eta_1 0\eta_{12}0\eta_2 0}(0,0;0,0,0) &= \int d^3x_2\int d^3x_1\frac{e^{-\eta_1x_1}}{x_1}\frac{e^{-\eta_{12}x_{12}}}{x_{12}}\frac{e^{-\eta_2x_2}}{x_2}. \\ &= \int_0^\infty dx_2 4\pi x_2^2\frac{4\pi(e^{-x_2\eta_{12}}-e^{-x_2\eta_1})}{x_2(\eta_1^2-\eta_{12}^2)}\frac{e^{-\eta_2x_2}}{x_2} \\ &= \frac{16\pi^2}{(\eta_1+\eta_2)(\eta_1+\eta_{12})(\eta_2+\eta_{12})} \end{aligned} \quad (39)$$

There is utility, however, in simultaneously transforming the full product of Slater orbitals to generate unusual integrals whose values we know (as above) but whose reduction path may be fraught with difficulty. If one can find the solution path for a known integral, this may provide a path for unknown integrals. Furthermore, it is clear that the integral representations of the present paper, like that in the prior paper, are unusual in that they have integration variables residing within square roots as the arguments of Macdonald functions.

The present integral representation appears on the surface to be less likely to allow for such a reduction because there are many fewer tabled integrals over the interval $[0,1]$ than there are over the $[0,\infty]$ interval in the integral representation of the prior work. We will see that this concern is not at all the case if we apply the strategy of doing both coordinate integrals first within the above integral.

We apply the integral representation Equation (28) to all three Slater orbitals simultaneously. After completing the square and changing variables, the integral over $x_1'^2 K_{\frac{3}{2}}\left(\alpha\sqrt{x_1'^2+z^2}\right)/\sqrt{\left(x_1'^2+z^2\right)^{3/2}}$ can be done using [21] (p. 727. No. 6.596.3), the consequent $x_2^2 K_0(\alpha x_2)$ integral can also be done via [28], and the second-to-last integral is given by [21] (p. 333 No. 3.194.1)

$$
\begin{aligned}
&S_1^{\eta_1 0\eta_{12}0\eta_2 0}(0,0;0,0,0) = \int d^3x_2 \int d^3x_1 \frac{e^{-\eta_1 x_1}}{x_1}\frac{e^{-\eta_{12}x_{12}}}{x_{12}}\frac{e^{-\eta_2 x_2}}{x_2} \\
&= \int d^3x_2 \int d^3x_1 \int_0^1 d\alpha_1 \int_0^1 d\sigma_2 \frac{\alpha_1\left((1-\alpha_1)\eta_1^2+\eta_{12}^2\alpha_1(1-\sigma_2)+\eta_2^2\alpha_1\sigma_2\right)^{3/4}}{\sqrt{2}\pi^{3/2}\left((1-\alpha_1)\alpha_1^2(1-\sigma_2)\sigma_2\right)^{3/2}} \\
&\times \frac{K_{\frac{3}{2}}\left(\sqrt{\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1(1-\sigma_2)}+\frac{x_2^2}{\alpha_1\sigma_2}}\sqrt{(1-\alpha_1)\eta_1^2+\eta_{12}^2\alpha_1(1-\sigma_2)+\eta_2^2\alpha_1\sigma_2}\right)}{\left(\frac{x_1^2}{1-\alpha_1}+\frac{x_{12}^2}{\alpha_1(1-\sigma_2)}+\frac{x_2^2}{\alpha_1\sigma_2}\right)^{3/4}} \\
&= \int d^3x_2 \int d^3x_1' \int_0^1 d\alpha_1 \int_0^1 d\sigma_2 \frac{\alpha_1\left((1-\alpha_1)\eta_1^2+\eta_{12}^2\alpha_1(1-\sigma_2)+\eta_2^2\alpha_1\sigma_2\right)^{3/4}}{\sqrt{2}\pi^{3/2}\left((1-\alpha_1)\alpha_1^2(1-\sigma_2)\sigma_2\right)^{3/2}} \\
&\times \frac{K_{\frac{3}{2}}\left(\sqrt{\frac{x_1'^2(1-\alpha_1\sigma_2)}{(1-\alpha_1)\alpha_1(1-\sigma_2)}+\frac{x_2^2}{\alpha_1\sigma_2-\alpha_1^2\sigma_2^2}}\sqrt{(1-\alpha_1)\eta_1^2+\eta_{12}^2\alpha_1(1-\sigma_2)+\eta_2^2\alpha_1\sigma_2}\right)}{\left(\frac{x_1'^2(1-\alpha_1\sigma_2)}{(1-\alpha_1)\alpha_1(1-\sigma_2)}+\frac{x_2^2}{\alpha_1\sigma_2-\alpha_1^2\sigma_2^2}\right)^{3/4}} \\
&= \int_0^\infty dx_2 \int_0^1 d\alpha_1 \int_0^1 d\sigma_2 8\pi x_2^2 K_0\left(\frac{x_2\sqrt{(1-\alpha_1)\eta_1^2+\alpha_1\eta_{13}^2\sigma_2+\eta_{12}^2(\alpha_1-\alpha_1\sigma_2)}}{\sqrt{\alpha_1}\sqrt{\sigma_2}\sqrt{1-\alpha_1\sigma_2}}\right) \\
&\times \frac{\left(\alpha_1\eta_{13}^2\sigma_2+\eta_{12}^2(\alpha_1-\alpha_1\sigma_2)+(1-\alpha_1)\eta_1^2\right)^{3/4}}{(1-\alpha_1)^{3/4}\alpha_1^{5/4}(1-\sigma_2)^{3/4}\sigma_2^{3/2}(1-\alpha_1\sigma_2)^{3/4}} \\
&\times \left(\frac{\sqrt{1-\alpha_1\sigma_2}\sqrt{\alpha_1\eta_{13}^2\sigma_2+\eta_{12}^2(\alpha_1-\alpha_1\sigma_2)+(1-\alpha_1)\eta_1^2}}{\sqrt{1-\alpha_1}\sqrt{\alpha_1}\sqrt{1-\sigma_2}}\right)^{-3/2} \\
&= \int_0^1 d\alpha_1 \int_0^1 d\sigma_2 \frac{4\pi^2\alpha_1}{\left(\alpha_1\left(\eta_{12}^2(1-\sigma_2)+\eta_{13}^2\sigma_2-\eta_1^2\right)+\eta_1^2\right)^{3/2}} \\
&= \int_0^1 d\sigma_2 \frac{8\pi^2\left(\sqrt{(\eta_{13}^2-\eta_{12}^2)\sigma_2+\eta_{12}^2}-\eta_1\right)^2}{\left((\eta_{12}^2-\eta_{13}^2)\sigma_2+\eta_1^2-\eta_{12}^2\right)^2\sqrt{(\eta_{13}^2-\eta_{12}^2)\sigma_2+\eta_{12}^2}} \\
&= \int_{\eta_{12}^2}^{\eta_{13}^2} \frac{8\pi^2}{\sqrt{y}(\eta_{13}^2-\eta_{12}^2)(\sqrt{y}+\eta_1)^2}dy = \int_{\eta_{12}}^{\eta_{13}} \frac{16\pi^2}{(\eta_{13}^2-\eta_{12}^2)(z+\eta_1)^2}dz \quad .
\end{aligned} \tag{40}
$$

Using [21] (p. 69 No. 2.113.1) in the final integral, above, gives the final line of Equation (39), and it does so in a more straightforward fashion—using tabled integrals—than did the integral representation of the prior paper when applied to this problem (which required the generation of new integrals in the final step using the computer algebra and calculus program Mathematica).

We will see next that this advantage over the prior method is not universal. That is, each integral representation, in turn, will shine brighter on specific problems.

The second general rule of analytical integration is that the easiest path is to integrate over the coordinate variables first. The doubly contrary approach of the prior paper generated a set of integrals that might be of utility for future researchers. We showed therein that integration (over the interval $[0,\infty]$), when the variables reside within square roots as the argument of a Macdonald function, can be undertaken if we rewrite the Macdonald function in terms of a Meijer G-function. In the case of a product of three Slater orbitals, after completing the square in the variable common to all three and then integrating over the result, one has the following function to be integrated over [29] (p. 665. No. 8.4.23.1):

$$\frac{1}{\zeta_2^{3/2}} K_0\left(2\frac{x_2\sqrt{\zeta_1+\zeta_2+1}\eta_2\sqrt{\frac{\zeta_1\eta_{12}^2+\eta_1^2}{4\eta_2^2}+\frac{\zeta_2}{4}}}{\sqrt{\zeta_1+1}\sqrt{\zeta_2}}\right) = \frac{1}{2}\frac{1}{\zeta_2^{3/2}} G_{0,2}^{2,0}\left(\frac{x_2^2(\zeta_1+\zeta_2+1)\eta_2^2\left(\zeta_2+\frac{\eta_1^2+\zeta_1\eta_{12}^2}{\eta_2^2}\right)}{(\zeta_1+1)\zeta_2}\mid\ 0,0\right), \tag{41}$$

for which there is but one tabled integral [29] (p. 349 No. 2.24.2.9) that has roughly the right form (with $\zeta_2 = x$),

$$\int_0^\infty dx\, x^{\alpha-1}\left(ax^2+bx+c\right)^{\frac{3}{2}-\alpha} G_{0,2}^{2,0}\left(\frac{ax^2+bx+c}{x}\mid\ \nu,-\nu\right) = \frac{\sqrt{\pi}G_{1,3}^{3,0}\left(b+2\sqrt{a}\sqrt{c}\mid\ {\frac{3}{2} \atop 0,-\alpha-\nu+3,-\alpha+\nu+3}\right)}{2a^{3/2}} + \frac{\sqrt{\pi}\sqrt{c}G_{1,3}^{3,0}\left(b+2\sqrt{a}\sqrt{c}\mid\ {\frac{1}{2} \atop 0,-\alpha-\nu+2,-\alpha+\nu+2}\right)}{a}. \tag{42}$$

A modification was required since inserting $\alpha = \frac{3}{2}$ to remove the polynomial multiplying the G-function in the integrand leaves us with the wrong power of x. One can, however, take derivatives with respect to c of the integrand and resultant, with $\nu = 1/2$ in combination with $\nu = 0$, to show the following (in Equation (43) and following, we explicitly include an alternative expression for K as the hypergeometric U function [30], while expressions in related functions can be found in [31,32] and [21] (p. 1090 No.9.235.2). None of these seem to have tabled integrals with arguments as complicated as [29] (p. 349 No. 2.24.2.9)):

$$\begin{aligned}
\int_0^\infty dx\,\frac{1}{x^{3/2}}K_0\left(2\sqrt{\frac{ax^2+bx+c}{x}}\right) &= \int_0^\infty dx\,\frac{1}{x^{3/2}}\sqrt{\pi}e^{-2\sqrt{\frac{ax^2+bx+c}{x}}}U\left(\frac{1}{2},1,4\sqrt{\frac{ax^2+bx+c}{x}}\right)\\
&= \int_0^\infty dx\,\frac{1}{2x^{3/2}}G_{0,2}^{2,0}\left(\frac{\mathrm{ax}^2+\mathrm{b\,x}+c}{x}\mid\ 0,0\right)\\
&= \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{2\sqrt{c}\sqrt{2\sqrt{a}\sqrt{c}+b}} - \frac{\sqrt{\pi}G_{1,3}^{2,1}\left(b+2\sqrt{a}\sqrt{c}\mid\ {-\frac{3}{2} \atop -\frac{1}{2},0,-\frac{1}{2}}\right)}{2\sqrt{c}},\\
&= \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{2\sqrt{c}}\\
&\Rightarrow \frac{\pi e^{-2\left(\frac{2\sqrt{a}\sqrt{c}}{x_2\eta_2}+\frac{x_2\eta_2}{2}\right)}}{2\sqrt{c}}
\end{aligned} \tag{43}$$

where the reduction of the Meijer G-function in the third line is from [33] and the last step

$$\sqrt{2\sqrt{a}\sqrt{c}+b} \Rightarrow \frac{2\sqrt{a}\sqrt{c}}{x_2\eta_2}+\frac{x_2\eta_2}{2} \tag{44}$$

holds for a number of cases akin to the present one in which

$$\left\{a \to \frac{x_2^2\eta_2^2}{4(\zeta_1+1)},\, b \to \frac{x_2^2\eta_2^2}{4(\zeta_1+1)}\left(\frac{\zeta_1\eta_{12}^2+\eta_1^2}{\eta_2^2}+\zeta_1+1\right),\, c \to \frac{1}{4}x_2^2\left(\zeta_1\eta_{12}^2+\eta_1^2\right)\right\} \quad . \tag{45}$$

The integral representations of the current paper use integrals over the interval $[0,1]$ rather than over $[0,\infty]$, and the only tabled integral over a G-function on $[0,1]$ we found that has a fairly complicated argument [29] (p. 349 No. 2.24.2.7),

$$\int_0^1 dx\, \frac{x^{\alpha-1}(1-x)^{\beta-1}}{(1+ax+b(1-x))^{\alpha+\beta}} G_{p,q}^{m,n}\left(\frac{x^\ell(1-x)^k}{(1+ax+b(1-x))^{\ell+k}}\middle| \begin{matrix}(a_p)\\(b_q)\end{matrix}\right) \tag{46}$$

has a markedly different integrand than the square of the argument of the Macdonald function

$$\frac{8\pi x_2^2}{\sqrt{\alpha_1}\sigma_2^{3/2}(1-\alpha_1\sigma_2)^{3/2}} K_0\left(\frac{x_2\sqrt{(1-\alpha_1)\eta_1^2+\alpha_1\eta_{13}^2\sigma_2+\eta_{12}^2(\alpha_1-\alpha_1\sigma_2)}}{\sqrt{\alpha_1}\sqrt{\sigma_2}\sqrt{1-\alpha_1\sigma_2}}\right) \tag{47}$$

to which the fourth equality in (40) reduces, so it is useless for the present problem.

Schweber's third parametrization gives no better result. All of this provided motivation for the integral representation we derive in the next section.

8. An Ungainly but Useful Bridge

There is an obscure integral [27] (p. 176 No. 421.8) that will serve as an integral representation for a product of denominators,

$$\begin{aligned}\frac{B(\kappa,\lambda-\kappa)}{c^\kappa d^{\lambda-\kappa}} &= \int_0^1 dx\left(\frac{x^{\kappa-1}}{(cx+d)^\lambda}+\frac{x^{-\kappa+\lambda-1}}{(c+dx)^\lambda}\right)=\int_1^\infty dx\left(\frac{x^{\kappa-1}}{(cx+d)^\lambda}+\frac{x^{-\kappa+\lambda-1}}{(c+dx)^\lambda}\right)\\ &= \frac{1}{2}\int_0^\infty dx\left(\frac{x^{\kappa-1}}{(cx+d)^\lambda}+\frac{x^{-\kappa+\lambda-1}}{(c+dx)^\lambda}\right) \quad ,\end{aligned} \tag{48}$$

that has the very useful property of relating integrals over $[0,\infty]$ to integrals over $[0,1]$ and $[1,\infty]$. One might hope to extend integrals like [29] (p. 349 No. 2.24.2.9) to integrals over $[0,1]$ or $[1,\infty]$ if the integral over $[0,\infty]$ could be found.

Its ungainliness is revealed in the process of extending it from a pair of denominators

$$\frac{1}{a_1a_2}=\int_0^1 d\tau_1\left(\frac{1}{(a_1+a_2\tau_1)^2}+\frac{1}{(a_1\tau_1+a_2)^2}\right) \tag{49}$$

to triplets by iteration

$$\begin{aligned}\frac{1}{a_1a_2a_3} &= \int_0^1 d\tau_1\int_0^1 d\tau_2\, 2\left(\frac{1}{(a_1\tau_1+a_3\tau_2+a_2)^3}+\frac{1}{(a_2\tau_1+a_3\tau_2+a_1)^3}\right.\\ &\left.+\frac{\tau_2}{(\tau_2(a_1\tau_1+a_2)+a_3)^3}+\frac{\tau_2}{(\tau_2(a_2\tau_1+a_1)+a_3)^3}\right)\end{aligned} \tag{50}$$

and beyond: at each step, the number of terms doubles so a general-M version is difficult to imagine.

To derive an integral representation for a product of two or three Slater orbitals, one simply follows the procedure laid out in Section 4, above, for each of the two or four terms, but the determinants are different in this new case and are different from term to term. The final forms are

$$\begin{aligned}\frac{e^{-\eta_1 x_1}}{x_1}\,\frac{e^{-\eta_{12} x_{12}}}{x_{12}} &= \int_0^1 d\tau_1 \int_0^\infty d\rho\, \frac{\exp\left(-\frac{\frac{x_1^2}{\tau_1}+x_{12}^2}{4\rho}-\rho\left(\eta_1^2\tau_1+\eta_{12}^2\right)\right)+\exp\left(-\frac{\frac{x_{12}^2}{\tau_1}+x_1^2}{4\rho}-\rho\left(\eta_{12}^2\tau_1+\eta_1^2\right)\right)}{4\pi\rho^2\tau_1^{3/2}} \\ &= \int_0^1 d\tau_1\left(\frac{\sqrt{\eta_1^2\tau_1+\eta_{12}^2}\,K_1\left(\sqrt{\frac{x_1^2}{\tau_1}+x_{12}^2}\sqrt{\tau_1\eta_1^2+\eta_{12}^2}\right)}{\pi\tau_1^{3/2}\sqrt{\frac{x_1^2}{\tau_1}+x_{12}^2}}+\frac{\sqrt{\eta_{12}^2\tau_1+\eta_1^2}\,K_1\left(\sqrt{x_1^2+\frac{x_{12}^2}{\tau_1}}\sqrt{\eta_1^2+\eta_{12}^2\tau_1}\right)}{\pi\tau_1^{3/2}\sqrt{\frac{x_{12}^2}{\tau_1}+x_1^2}}\right)\end{aligned} \tag{51}$$

and

$$\begin{aligned}\frac{e^{-\eta_1 x_1}}{x_1}\,\frac{e^{-\eta_{12} x_{12}}}{x_{12}}\,\frac{e^{-\eta_{13} x_{13}}}{x_{13}} &= \int_0^1 d\tau_1 \int_0^1 d\tau_2 \int_0^\infty d\rho\,\frac{1}{8\pi^{3/2}\rho^{5/2}(\tau_1\tau_2)^{3/2}} \\ &+ \left[\exp\left(-\frac{\frac{x_1^2}{\tau_1}+\frac{x_{13}^2}{\tau_2}+x_{12}^2}{4\rho}-\rho\left(\eta_1^2\tau_1+\eta_{13}^2\tau_2+\eta_{12}^2\right)\right)\right. \\ &+ \exp\left(-\frac{\frac{x_{12}^2}{\tau_1}+\frac{x_{13}^2}{\tau_2}+x_1^2}{4\rho}-\rho\left(\eta_{12}^2\tau_1+\eta_{13}^2\tau_2+\eta_1^2\right)\right) \\ &+ \tau_2\exp\left(-\frac{\frac{x_1^2}{\tau_1\tau_2}+\frac{x_{12}^2}{\tau_2}+x_{13}^2}{4\rho}-\rho\left(\eta_1^2\tau_1\tau_2+\eta_{12}^2\tau_2+\eta_{13}^2\right)\right) \\ &+ \left.\tau_2\exp\left(-\frac{\frac{x_1^2}{\tau_2}+\frac{x_{12}^2}{\tau_1\tau_2}+x_{13}^2}{4\rho}-\rho\left(\eta_1^2\tau_2+\eta_{12}^2\tau_1\tau_2+\eta_{13}^2\right)\right)\right] \\ &= \int_0^1 d\tau_1\int_0^1 d\tau_2\left(\frac{\left(\eta_1^2\tau_1+\eta_{13}^2\tau_2+\eta_{12}^2\right)^{3/4}K_{\frac{3}{2}}\left(\sqrt{\frac{x_1^2}{\tau_1}+x_{12}^2+\frac{x_{13}^2}{\tau_2}}\sqrt{\tau_1\eta_1^2+\eta_{12}^2+\eta_{13}^2\tau_2}\right)}{\sqrt{2}\pi^{3/2}(\tau_1\tau_2)^{3/2}\left(\frac{x_1^2}{\tau_1}+\frac{x_{13}^2}{\tau_2}+x_{12}^2\right)^{3/4}}\right. \\ &+ \frac{\left(\eta_{12}^2\tau_1+\eta_{13}^2\tau_2+\eta_1^2\right)^{3/4}K_{\frac{3}{2}}\left(\sqrt{x_1^2+\frac{x_{12}^2}{\tau_1}+\frac{x_{13}^2}{\tau_2}}\sqrt{\eta_1^2+\eta_{12}^2\tau_1+\eta_{13}^2\tau_2}\right)}{\sqrt{2}\pi^{3/2}(\tau_1\tau_2)^{3/2}\left(\frac{x_{12}^2}{\tau_1}+\frac{x_{13}^2}{\tau_2}+x_1^2\right)^{3/4}} \\ &\quad \frac{\left(\eta_1^2\tau_1\tau_2+\eta_{12}^2\tau_2+\eta_{13}^2\right)^{3/4}K_{\frac{3}{2}}\left(\sqrt{\frac{x_1^2}{\tau_1\tau_2}+x_{13}^2+\frac{x_{12}^2}{\tau_2}}\sqrt{\tau_1\tau_2\eta_1^2+\eta_{13}^2+\eta_{12}^2\tau_2}\right)}{\sqrt{2}\pi^{3/2}\tau_1^{3/2}\tau_2^2\left(\frac{x_1^2}{\tau_1\tau_2}+\frac{x_{12}^2}{\tau_2}+x_{13}^2\right)^{3/4}} \\ &+ \left.\frac{\left(\eta_1^2\tau_2+\eta_{12}^2\tau_1\tau_2+\eta_{13}^2\right)^{3/4}K_{\frac{3}{2}}\left(\sqrt{\frac{x_1^2}{\tau_2}+x_{13}^2+\frac{x_{12}^2}{\tau_1\tau_2}}\sqrt{\tau_2\eta_1^2+\eta_{13}^2+\eta_{12}^2\tau_1\tau_2}\right)}{\sqrt{2}\pi^{3/2}\tau_1^{3/2}\tau_2^2\left(\frac{x_1^2}{\tau_2}+\frac{x_{12}^2}{\tau_1\tau_2}+x_{13}^2\right)^{3/4}}\right)\end{aligned}, \tag{52}$$

with the equality also holding for integrals over $[1,\infty]$. It also holds over $[0,\infty]$ if one multiplies the right-hand side by $\frac{1}{2}\frac{1}{2}$. In the case of $M \geq 3$, one can even mix these three intervals among the integrals present.

We (simultaneously) apply the above integral representation (52) to all three Slater orbitals in the first line of (39), whose last line gives 117.4952904891590 when we arbitrarily set parameters to $\{\eta_1 \to 0.3, \eta_{12} \to 0.5,\ \ \eta_{13} \to 0.9\}$. After completing the square and changing variables, using [21] (p. 727. No. 6.596.3), one can perform the integral over $x_1'^2 K_{\frac{3}{2}}\left(\alpha\sqrt{x_1'^2+z^2}\right)/\sqrt{\left(x_1'^2+z^2\right)^{3/2}}$.

$$S_1^{\eta_1 0\eta_{12} 0\eta_2 0}(0,0;0,0,0)=\int d^3x_2\int d^3x_1\frac{e^{-\eta_1x_1}}{x_1}\frac{e^{-\eta_{12}x_{12}}}{x_{12}}\frac{e^{-\eta_2x_2}}{x_2}=\int d^3x_2\int d^3x_1'\int_0^1 d\tau_1\int_0^1 d\tau_2$$
$$\times\left(\frac{(\eta_1^2\tau_1+\eta_{13}^2\tau_2+\eta_{12}^2)^{3/4}K_{\frac{3}{2}}\left(\sqrt{\frac{x_1'^2(\tau_1+1)}{\tau_1}+\frac{x_2^2(\tau_1+\tau_2+1)}{(\tau_1+1)\tau_2}}\sqrt{\tau_1\eta_1^2+\eta_{12}^2+\eta_{13}^2\tau_2}\right)}{\sqrt{2}\pi^{3/2}(\tau_1\tau_2)^{3/2}\left(\frac{x_1'^2(\tau_1+1)}{\tau_1}+\frac{x_2^2(\tau_1+\tau_2+1)}{(\tau_1+1)\tau_2}\right)^{3/4}}\right.$$
$$+\frac{(\eta_{12}^2\tau_1+\eta_{13}^2\tau_2+\eta_1^2)^{3/4}K_{\frac{3}{2}}\left(\sqrt{\frac{x_1'^2(\tau_1+1)}{\tau_1}+\frac{x_2^2(\tau_1+\tau_2+1)}{(\tau_1+1)\tau_2}}\sqrt{\eta_1^2+\eta_{12}^2\tau_1+\eta_{13}^2\tau_2}\right)}{\sqrt{2}\pi^{3/2}(\tau_1\tau_2)^{3/2}\left(\frac{x_1'^2(\tau_1+1)}{\tau_1}+\frac{x_2^2(\tau_1+\tau_2+1)}{(\tau_1+1)\tau_2}\right)^{3/4}}$$
$$+\frac{(\eta_1^2\tau_1\tau_2+\eta_{12}^2\tau_2+\eta_{13}^2)^{3/4}K_{\frac{3}{2}}\left(\sqrt{\frac{x_1'^2(\tau_1+1)}{\tau_1\tau_2}+\frac{x_2^2((\tau_1+1)\tau_2+1)}{(\tau_1+1)\tau_2}}\sqrt{\tau_1\tau_2\eta_1^2+\eta_{13}^2+\eta_{12}^2\tau_2}\right)}{\sqrt{2}\pi^{3/2}\tau_1^{3/2}\tau_2^2\left(\frac{x_1'^2(\tau_1+1)}{\tau_1\tau_2}+\frac{x_2^2((\tau_1+1)\tau_2+1)}{(\tau_1+1)\tau_2}\right)^{3/4}}$$
$$\left.+\frac{(\eta_1^2\tau_2+\eta_{12}^2\tau_1\tau_2+\eta_{13}^2)^{3/4}K_{\frac{3}{2}}\left(\sqrt{\frac{x_1'^2(\tau_1+1)}{\tau_1\tau_2}+\frac{x_2^2((\tau_1+1)\tau_2+1)}{(\tau_1+1)\tau_2}}\sqrt{\tau_2\eta_1^2+\eta_{13}^2+\eta_{12}^2\tau_1\tau_2}\right)}{\sqrt{2}\pi^{3/2}\tau_1^{3/2}\tau_2^2\left(\frac{x_1'^2(\tau_1+1)}{\tau_1\tau_2}+\frac{x_2^2((\tau_1+1)\tau_2+1)}{(\tau_1+1)\tau_2}\right)^{3/4}}\right)$$
$$=\int d^3x_2\int_0^1 d\tau_1\int_0^1 d\tau_2\left(\frac{2K_0\left(\frac{x_2\sqrt{\tau_1+\tau_2+1}\sqrt{\tau_1\eta_1^2+\eta_{12}^2+\eta_{13}^2\tau_2}}{\sqrt{\tau_1+1}\sqrt{\tau_2}}\right)}{(\tau_1+1)^{3/2}\tau_2^{3/2}}\right.$$
$$+\frac{2K_0\left(\frac{x_2\sqrt{\tau_1+\tau_2+1}\sqrt{\eta_1^2+\eta_{12}^2\tau_1+\eta_{13}^2\tau_2}}{\sqrt{\tau_1+1}\sqrt{\tau_2}}\right)}{(\tau_1+1)^{3/2}\tau_2^{3/2}}$$
$$\left.+\frac{2K_0\left(\frac{x_2\sqrt{\tau_1\tau_2\eta_1^2+\eta_{13}^2+\eta_{12}^2\tau_2}\sqrt{(\tau_1+1)\tau_2+1}}{\sqrt{\tau_1+1}\sqrt{\tau_2}}\right)}{(\tau_1+1)^{3/2}\sqrt{\tau_2}}+\frac{2K_0\left(\frac{x_2\sqrt{\tau_2\eta_1^2+\eta_{13}^2+\eta_{12}^2\tau_1\tau_2}\sqrt{(\tau_1+1)\tau_2+1}}{\sqrt{\tau_1+1}\sqrt{\tau_2}}\right)}{(\tau_1+1)^{3/2}\sqrt{\tau_2}}\right). \tag{53}$$

For the values of $\{\eta_1\to 0.3,\eta_{12}\to 0.5,\eta_{13}\to 0.9\}$ used above, these four terms numerically integrate to

$$S_1^{0.3,0,0.5,0,0.9,0}(0,0;0,0,0)=(39.2072+61.8386+7.89946+8.55004)=117.49528665800858\,. \tag{54}$$

On the other hand, if we change the integration limits to $[1,\infty]$, they yield

$$S_1^{0.3,0,0.5,0,0.9,0}(0,0;0,0,0)=(31.4147+22.115+38.9735+24.9916)=117.49480820934275\,. \tag{55}$$

If we now change the integration limits to $[0,\infty]$ and multiply by $\frac{1}{2}\frac{1}{2}$, these terms are

$$\begin{aligned}S_1^{0.3,0,0.5,0,0.9,0}&(0,0;0,0,0)=\\ =\;&(29.373735823279375+29.37376872163303\\ +\;&29.373735823279382+29.37376872163304)=117.49500908982483\quad.\end{aligned} \tag{56}$$

It should not be surprising that changing the limits of integration will change the value of an integral, nor that different integrands will yield different results under changed limits of integration. What is remarkable is that the four different integrands in each case compensate for each other under such a change of integration limits so as to produce the same sum (to six-digit accuracy in this numerical integration) for all three limit sets. (Such compensation is inherent in the integral representation (49) we used as the stepping stone to the Slater orbital version expressed in Equations (51) and (52).) This compensation is also a harbinger of the $[0, \infty]$ form of the present set of integral representations indeed acting as a bridge to analytical results for *sums* of integrals of Meijer G-functions over the intervals $[0, 1]$ and $[1, \infty]$. It is also notable that the four terms contribute almost equally when the limits are set to $[0, \infty]$, with the first and third terms the same to 15 digits—as are the second and fourth—though the first and second terms differ in the 7th digit.

9. Analytical Results for Sums of Integrals of Such G-Functions

Rather than doing the $x_2^2 K_0(a x_2)$ integrals via [28], we will attempt to do the τ_2 integrals first as a means to generate some useful integrals for future researchers. We begin by recasting the Macdonald functions of (53) as Meijer G-functions using (41) [29] (p. 665. No. 8.4.23.1), with each of the four terms having different values for

$$\begin{array}{l} \left\{a \to \frac{x_2^2 \eta_{13}^2}{4(\tau_1+1)},\, b \to \frac{x_2^2\left(\eta_1^2 \tau_1 + \eta_{13}^2(\tau_1+1) + \eta_{12}^2\right)}{4(\tau_1+1)},\, c \to \frac{1}{4} x_2^2\left(\eta_1^2 \tau_1 + \eta_{12}^2\right)\right\} \\ \left\{a_2 \to \frac{x_2^2 \eta_{13}^2}{4(\tau_1+1)},\, b_2 \to \frac{x_2^2\left(\eta_{12}^2 \tau_1 + \eta_{13}^2(\tau_1+1) + \eta_1^2\right)}{4(\tau_1+1)},\, c_2 \to \frac{1}{4} x_2^2\left(\eta_{12}^2 \tau_1 + \eta_1^2\right)\right\} \\ \left\{a_3 \to \frac{1}{4} x_2^2\left(\eta_1^2 \tau_1 + \eta_{12}^2\right),\, b_3 \to \frac{x_2^2\left(\eta_1^2 \tau_1 + \eta_{13}^2(\tau_1+1) + \eta_{12}^2\right)}{4(\tau_1+1)},\, c_3 \to \frac{x_2^2 \eta_{13}^2}{4(\tau_1+1)}\right\} \\ \left\{a_4 \to \frac{1}{4} x_2^2\left(\eta_{12}^2 \tau_1 + \eta_1^2\right),\, b_4 \to \frac{x_2^2\left(\eta_{12}^2 \tau_1 + \eta_{13}^2(\tau_1+1) + \eta_1^2\right)}{4(\tau_1+1)},\, c_4 \to \frac{x_2^2 \eta_{13}^2}{4(\tau_1+1)}\right\} \end{array} . \tag{57}$$

We switch to the form with integrals over $[0, \infty]$ so that we can consider just the first term of (53) that is precisely the integral found in the prior paper's Equation (43) except that in the present case, with $\left\{a \to \frac{x_2^2 \eta_{13}^2}{4(\tau_1+1)},\, b \to \frac{x_2^2\left(\eta_1^2 \tau_1 + \eta_{13}^2(\tau_1+1) + \eta_{12}^2\right)}{4(\tau_1+1)},\, c \to \frac{1}{4} x_2^2\left(\eta_1^2 \tau_1 + \eta_{12}^2\right)\right\}$, the last term simplifies differently:

$$\sqrt{2\sqrt{a}\sqrt{c} + b} \Rightarrow \sqrt{a(\tau_1 + 1)} + 2\sqrt{\frac{c}{\tau_1 + 1}} \quad . \tag{58}$$

Then,

$$\begin{array}{rr} \int d^3x_2 \frac{1}{2^2} \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \frac{2}{(\tau_1+1)^{3/2} \tau_2^{3/2}} K_0\left(\frac{2\sqrt{\frac{\eta_{13}^2 \tau_2^2 x_2^2}{4(\tau_1+1)} + \frac{1}{4}\left(\tau_1 \eta_1^2 + \eta_{12}^2\right) x_2^2 + \frac{\left(\tau_1 \eta_1^2 + \eta_{12}^2 + \eta_{13}^2(\tau_1+1)\right) \tau_2 x_2^2}{4(\tau_1+1)}}}{\sqrt{\tau_2}}\right) & = \\ \int d^3x_2 \frac{1}{2} \frac{1}{2} \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \frac{1}{(\tau_1+1)^{3/2}} \frac{2}{\tau_2^{3/2}} K_0\left(2 \frac{\sqrt{a\tau_2^2 + b\tau_2 + c}}{\sqrt{\tau_2}}\right) & = \\ \int d^3x_2 \frac{1}{2} \frac{1}{2} \int_0^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{\sqrt{c}} & \Rightarrow \\ \int d^3x_2 \frac{1}{2} \frac{1}{2} \int_0^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)} + \sqrt{\frac{c}{\tau_1+1}}\right)} & \end{array} \tag{59}$$

The second term has the same general form but with η_1^2 and η_{12}^2 switching places in their associations with τ_1 (symbolically, $\eta_1^2 \leftrightarrow \eta_{12}^2$). This means that we can write it as

$$\begin{aligned}\int d^3x_2 \frac{1}{2^2} \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \frac{2}{(\tau_1+1)^{3/2}\tau_2^{3/2}} K_0\left(\frac{2\sqrt{\frac{\eta_{13}^2\tau_2^2x_2^2}{4(\tau_1+1)}+\frac{1}{4}\left(\eta_1^2+\eta_{12}^2\tau_1\right)x_2^2+\frac{\left(\eta_1^2+\eta_{12}^2\tau_1+\eta_{13}^2(\tau_1+1)\right)\tau_2x_2^2}{4(\tau_1+1)}}}{\sqrt{\tau_2}}\right) &= \\ \int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \frac{1}{(\tau_1+1)^{3/2}} \frac{2}{\tau_2^{3/2}} K_0\left(2\frac{\sqrt{a\tau_2^2+(b-f)\tau_2+(c-g)}}{\sqrt{\tau_2}}\right) &= \\ \int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c-g}+(b-f)}}}{\sqrt{c-g}} &\Rightarrow \\ \int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}+\sqrt{\frac{c-g}{\tau_1+1}}\right)} &\end{aligned} \tag{60}$$

where

$$\left\{ g \to \frac{1}{4}x_2^2\left(\eta_1^2-\eta_{12}^2\right)(\tau_1-1), f \to \frac{x_2^2(\eta_1^2-\eta_{12}^2)(\tau_1-1)}{4(\tau_1+1)} \right\} \tag{61}$$

The third term has $x^{1/2}$ instead of $x^{3/2}$ in the denominator so we have to use a different sequence of derivatives of (42) to find that

$$\begin{aligned}\int_0^\infty dx \frac{1}{x^{1/2}} K_0\left(2\sqrt{\frac{ax^2+bx+c}{x}}\right) &= \int_0^\infty dx \frac{1}{x^{1/2}} \sqrt{\pi} e^{-2\sqrt{\frac{ax^2+bx+c}{x}}} U\left(\frac{1}{2}, 1, 4\sqrt{\frac{ax^2+bx+c}{x}}\right) \\ &= \int_0^\infty dx \frac{1}{2x^{1/2}} G_{0,2}^{2,0}\left(\frac{\mathrm{ax}^2+\mathrm{b\,x}+c}{x} \middle| \; 0,0 \right) \\ &= \frac{\sqrt{\pi}}{\sqrt{a}} G_{1,3}^{3,0}\left(b+2\sqrt{a}\sqrt{c} \middle| \begin{matrix} -\frac{1}{2} \\ 0, -\frac{1}{2}, \frac{1}{2} \end{matrix}\right) \quad , \\ &= \frac{e^{-2\sqrt{b+2\sqrt{a}\sqrt{c}}}\pi}{\sqrt{a}} \\ &\Rightarrow \frac{\pi}{\sqrt{a_3}} e^{-2\left(\sqrt{\frac{a_3}{\tau_1+1}}+\sqrt{c_3(\tau_1+1)}\right)}\end{aligned} \tag{62}$$

where the reduction in the fourth line is from [34] and the last line holds for the class of parameters akin to this particular set: $\left\{ a_3 \to \frac{1}{4}x_2^2(\eta_1^2\tau_1+\eta_{12}^2),\, b_3 \to \frac{x_2^2\left(\eta_1^2\tau_1+\eta_{13}^2(\tau_1+1)+\eta_{12}^2\right)}{4(\tau_1+1)},\right.$ $\left. c_3 \to \frac{x_2^2\eta_{13}^2}{4(\tau_1+1)} \right\}$. We furthermore see that $\{a_3 \to c,\, c_3 \to a\}$ in the present case, so the third term integrates to the same value as the first:

$$\begin{aligned}\int d^3x_2 \frac{1}{2^2} \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \frac{2}{(\tau_1+1)^{3/2}\sqrt{\tau_2}} K_0\left(\frac{2\sqrt{\frac{1}{4}\left(\tau_1\eta_1^2+\eta_{12}^2\right)\tau_2^2x_2^2+\frac{\left(\tau_1\eta_1^2+\eta_{12}^2+\eta_{13}^2(\tau_1+1)\right)\tau_2x_2^2}{4(\tau_1+1)}+\frac{\eta_{13}^2x_2^2}{4(\tau_1+1)}}}{\sqrt{\tau_2}}\right) &= \\ \int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \frac{1}{(\tau_1+1)^{3/2}} \frac{2}{\sqrt{\tau_2}} K_0\left(\frac{2\sqrt{c\tau_2^2+b\tau_2+a}}{\sqrt{\tau_2}}\right) &= \\ \int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{\sqrt{c}} &\Rightarrow \\ \int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}+\sqrt{\frac{c}{\tau_1+1}}\right)} &\end{aligned} \tag{63}$$

The fourth term has the same general form as the third but with $\eta_1^2 \leftrightarrow \eta_{12}^2$. This means that we can write it as

$$
\begin{aligned}
&\int d^3x_2 \frac{1}{2^2} \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \frac{2}{(\tau_1+1)^{3/2}\tau_2^{1/2}} K_0\left(\frac{2\sqrt{\frac{1}{4}\left(\eta_1^2+\eta_{12}^2\tau_1\right)\tau_2^2 x_2^2+\frac{\left(\eta_1^2+\eta_{12}^2\tau_1+\eta_{13}^2(\tau_1+1)\right)\tau_2 x_2^2}{4(\tau_1+1)}+\frac{\eta_{13}^2 x_2^2}{4(\tau_1+1)}}}{\sqrt{\tau_2}}\right) &&= \\
&\int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \frac{1}{(\tau_1+1)^{3/2}} \frac{2}{\tau_2^{1/2}} K_0\left(2\frac{\sqrt{a\tau_2^2+(b-f)\tau_2+(c-g)}}{\sqrt{\tau_2}}\right) &&= \\
&\int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c-g}+(b-f)}}}{\sqrt{c-g}} = &&\Rightarrow \\
&\int d^3x_2 \frac{1}{2}\frac{1}{2} \int_0^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}-\sqrt{\frac{c-g}{\tau_1+1}}\right)}
\end{aligned}
\tag{64}
$$

where f and g are as in (61).

In numerically integrating these final four analytical results, the final lines of (59), (60), (63), and (64), for the values of $\{\eta_1 \to 0.3, \eta_{12} \to 0.5, \eta_{13} \to 0.9\}$ used above, the four terms differ only in the final two decimal places:

$$
\begin{aligned}
S_1^{0.3,0,0.5,0,0.9,0}(0,0;0,0,0) &= (29.37382253070293 + 29.373822530702924 \\
+ &\quad 29.37382253070293 + 29.373822530702924) \\
= &\quad 117.49529012281171 \quad ,
\end{aligned}
\tag{65}
$$

and the penultimate lines in each case are identically 29.373822530702924. So our hope that the sum of the four integrals over the intervals $[0,1]$ and $[1,\infty]$ could be analytically found by using integration limits of $[0,\infty]$ as a sort of Rosetta stone bears fruit:

$$
\begin{aligned}
&\int d^3x_2 \int_1^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \int_1^\infty d\tau_2 \left(\frac{2}{\tau_2^{3/2}}\left[K_0\left(2\frac{\sqrt{a\tau_2^2+b\tau_2+c}}{\sqrt{\tau_2}}\right)+K_0\left(2\frac{\sqrt{a\tau_2^2+(b-f)\tau_2+(c-g)}}{\sqrt{\tau_2}}\right)\right]\right. &&+ \\
&\left.\frac{2}{\sqrt{\tau_2}}\left[K_0\left(\frac{2\sqrt{c\tau_2^2+b\tau_2+a}}{\sqrt{\tau_2}}\right)+K_0\left(2\frac{\sqrt{a\tau_2^2+(b-f)\tau_2+(c-g)}}{\sqrt{\tau_2}}\right)\right]\right) &&= \\
&31.4147 + 22.115 + 38.9735 + 24.9916 = 117.495 &&= \\
&\int d^3x_2 \int_1^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \left(\frac{\pi}{\sqrt{c}} e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}} + \frac{\pi}{\sqrt{c-g}} e^{-2\sqrt{2\sqrt{a}\sqrt{c-g}+(b-f)}}\right. &&+ \\
&\left.\frac{\pi}{\sqrt{c}} e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}} + \frac{\pi}{\sqrt{c-g}} e^{-2\sqrt{2\sqrt{a}\sqrt{c-g}+(b-f)}}\right) &&\Rightarrow \quad . \\
&\int d^3x_2 \int_1^\infty d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \left(\frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}-\sqrt{\frac{c}{\tau_1+1}}\right)} + \frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}-\sqrt{\frac{c-g}{\tau_1+1}}\right)}\right. &&+ \\
&\left.\frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}+\sqrt{\frac{c}{\tau_1+1}}\right)} + \frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}-\sqrt{\frac{c-g}{\tau_1+1}}\right)}\right) &&= \\
&35.1943 + 23.5533 + 35.1943 + 23.5533 = 117.495
\end{aligned}
\tag{66}
$$

We note that the analytical τ_2 results (in the last line above after numerically integrating over $d^3x_2 d\tau_1$) are identical for the first and third terms and for the second and fourth. One can likewise see that the average of the first and third terms resulting from the numerical integral that includes $d\tau_2$ (in the third line above) gives the first analytical term, and the average of the second and fourth terms resulting from the numerical integral that includes $d\tau_2$ gives the second analytical term. So our results extend significantly beyond our hope that the sum of the four integrals over the interval $[1,\infty]$ would have an analytical result. In fact, an analytical result comes from the sum of only two terms. The same holds when we replace the integral limits with $[0,1]$. Written with this new understanding, the pairs of integrals give

$$
\begin{aligned}
\int d^3x_2 \int_0^1 d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \int_0^1 d\tau_2 \left(\frac{2}{\tau_2^{3/2}} K_0\left(2\frac{\sqrt{a\tau_2^2+b\tau_2+c}}{\sqrt{\tau_2}}\right) + \frac{2}{\sqrt{\tau_2}} K_0\left(\frac{2\sqrt{c\tau_2^2+b\tau_2+a}}{\sqrt{\tau_2}}\right)\right) &= \\
\int d^3x_2 \int_0^1 d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \frac{\pi}{\sqrt{c}} e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}} &\Rightarrow \\
\int d^3x_2 \int_0^1 d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} 2\frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}-\sqrt{\frac{c}{\tau_1+1}}\right)} &= \\
2\times 23.5533 & \\
\int d^3x_2 \int_0^1 d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} \int_0^1 d\tau_2 \left(\frac{2}{\tau_2^{3/2}} K_0\left(2\frac{\sqrt{a\tau_2^2+(b-f)\tau_2+(c-g)}}{\sqrt{\tau_2}}\right)\right. &+ \\
\left. + \frac{2}{\sqrt{\tau_2}} K_0\left(2\frac{\sqrt{a\tau_2^2+(b-f)\tau_2+(c-g)}}{\sqrt{\tau_2}}\right)\right) &= \\
\int d^3x_2 \int_0^1 d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} 2\frac{\pi}{\sqrt{c-g}} e^{-2\sqrt{2\sqrt{a}\sqrt{c-g}+(b-f)}} &\Rightarrow \\
\int d^3x_2 \int_0^1 d\tau_1 \frac{1}{(\tau_1+1)^{3/2}} 2\frac{\pi}{\sqrt{c}} e^{-2\left(\sqrt{a(\tau_1+1)}-\sqrt{\frac{c-g}{\tau_1+1}}\right)} &= \\
2\times 35.1943 &
\end{aligned} \tag{67}
$$

whose sum is again 117.495.

We noted earlier that one can have a different τ_1 integration interval than for τ_2. If we substitute $[0,\infty]$ for the τ_1 integration interval and multiply by $\frac{1}{2}$ while keeping $[0,1]$ for the τ_2 integral, each of the above two integrals yields a value of 2×29.3738 whose sum is again 117.495. These are averages of the first and third terms in the set of results from the individual terms {39.0904, 43.4151, 19.6571, 15.3325}. The same holds if we substitute $[0,\infty]$ for the τ_1 integration interval and multiply by $\frac{1}{2}$ while setting $[1,\infty]$ for the τ_2 integral, though the first and last pairs swap values in the individual terms.

These are integral results extracted from the particular case under study. Of course, the final form will not hold for generic values of the parameters, but do the penultimate ones hold? Indeed, they do:

$$
\begin{aligned}
\int_0^1 dx\left(\frac{2}{x^{3/2}}K_0\left(\frac{2\sqrt{ax^2+bx+c}}{\sqrt{x}}\right) + \frac{2}{\sqrt{x}}K_0\left(\frac{2\sqrt{cx^2+bx+a}}{\sqrt{x}}\right)\right) &= \\
\int_0^1 dx\left(\frac{2\sqrt{\pi}}{x^{3/2}}e^{-\frac{2\sqrt{ax^2+bx+c}}{\sqrt{x}}}U\left(\frac{1}{2},1,\frac{4\sqrt{ax^2+bx+c}}{\sqrt{x}}\right) + \frac{2\sqrt{\pi}}{\sqrt{x}}e^{-\frac{2\sqrt{a+bx+cx^2}}{\sqrt{x}}}U\left(\frac{1}{2},1,\frac{4\sqrt{cx^2+bx+a}}{\sqrt{x}}\right)\right) &= \\
\int_0^1 dx\left(\frac{1}{x^{3/2}}G_{0,2}^{2,0}\left(\frac{ax^2+bx+c}{x}\middle|\ 0,0\right) + \frac{1}{\sqrt{x}}G_{0,2}^{2,0}\left(\frac{cx^2+bx+a}{x}\middle|\ 0,0\right)\right) &= \\
\frac{\pi}{\sqrt{c}}e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}} &= \\
0.738215 & \\
[\{a\to 0.21,\ b\to 0.31,\ c\to 0.41\}] &
\end{aligned} \tag{68}
$$

The same values result when the integration is over the interval $[1,\infty]$ as they do if we change the integration limits to $[0,\infty]$ and multiply by $\frac{1}{2}$. We note that the second pair of integrals in (67), when cast into generic terms, replicate the above integral if we simply rename $b-f$ as b and $c-g$ as g, so we have derived one new integral relation and not two distinct ones.

While each of the two terms in the above integral does not map onto a known analytical result, having the sum map onto a known analytical result is a significant step in that direction.

10. Conclusions

We crafted a quartet of integral representations of products of Slater orbitals over the interval $[0,1]$ that may be useful in the reduction of multidimensional transition amplitudes of quantum theory. For three of these representations, the general form was found for a product of any number of Slater orbitals, whose derivatives in the atomic realm represent hydrogenic and Hylleraas wave functions, as well as those composed of explicitly correlated exponentials of the kind introduced by Thakkar and Smith [35]. These results are also useful in nuclear transition amplitudes and may also find application in solid-state physics, plasma physics, negative ion physics, and problems involving a hypothesized non-zero-mass photon.

These three integral representations have the advantage over the Gaussian transform of requiring the introduction of one fewer integral to be subsequently reduced. They also require many fewer than the $(3(M-1)+M-1)$ integral dimensions that the Fourier transform introduces for a product of M Slater orbitals. Direct integration of products of Slater orbitals containing angular functions centered on different points usually bears fruit in only the simplest problems. The fourth conventional approach to these problems is to represent M Slater orbitals as M addition theorems, that is, M infinite sums over spherical harmonics containing the angular dependencies. Orthogonality allows one to remove a few of these infinite sums in the process of integrating some of the original integrals. For large M, this approach rapidly bogs down.

Each of the four extant approaches to such problems runs into difficulties at some point as M increases. These three new integral representations (over the interval $[0,1]$) for M Slater orbitals likewise have some positives and some negatives. One advantage for numerical integration using the present set compared to undertaking this integration with the version in the prior paper—which has integrals running over the interval $[0,\infty]$ (as do and Fourier and Gaussian methods)—is avoiding the inconvenience of needing to test for a sufficiently large upper integration limit.

For the simplest analytical integration problems, the three integral representations (over the interval $[0,1]$) for Slater orbitals in the present paper provide solutions in a much more rapid fashion than do the four traditional approaches and even surpass the integral representation over the interval $[0,\infty]$ of the prior paper in allowing the moderately hard problem of the integral over three Slater orbitals—after all coordinate integrals have been performed—to be reduced to analytical form via tabled integrals over the interval $[0,1]$. On the other hand, the integral representation over the interval $[0,\infty]$ of the prior paper lacked any tabled result in the final step of this problem and had to rely on the computer algebra and calculus program Mathematica 7 to find this integral. This, however, belies the general paucity of tabled integrals over the interval $[0,1]$ relative to those over the interval $[0,\infty]$.

The fact that the integration variables reside within a square root as the argument of a Macdonald function, shared by the prior work, will lead to difficulties in some complicated problems since only one such integral (transformed into a Meijer G-function) was known before extensions in the prior paper. Unlike that paper, the three integral representations for M Slater orbitals of the present work have the added difficulty of having no known integrals of this sort upon which to build.

It was for this reason that we introduced a fourth integral representation that is not easily generalizable to large M, but we hoped it would provide a bridge for finding the requisite integrals in the above problems. This final integral representation allowed us to derive the analytical result for an integral of a *sum of two* Meijer G-functions $f(x)G_{0,2}^{2,0}\left(\frac{\mathrm{ax}^2+\mathrm{b\,x}+c}{x}\middle|\ 0,0\right)$ over the interval $[0,1]$ via a bridge from the version of this integral representation that is over the interval $[0,\infty]$. This is only halfway to the desired result but is a promising step and provides an integral that researchers in fields far afield from atomic theory may find useful.

Funding: This research received no external funding.

Data Availability Statement: Data are contained within the article.

Acknowledgments: As it became clear that I needed to make at least some progress on finding analytical results for integrals of Meijer G-functions $f(x)G_{0,2}^{2,0}\left(\frac{\mathrm{ax}^2+\mathrm{b\,x}+c}{x}\middle|\ 0,0\right)$ over the interval $[0,1]$ for this research project to come to a sense of completion, I chanced upon an integral in Gröbner and Hofreiter [27] (p. 176 No. 421.8) that would serve as an integral representation for a product of denominators. I found that I could use this as the basis for an integral representation for a product of

several Slater orbitals that had the property of bridging from known integrals of Meijer G-functions (with such arguments) over the interval $[0, \infty]$ to heretofore untabled pairs of such integrals over the the interval $[0, 1]$ (and over $[1, \infty]$)—a sort of mathematical Rosetta stone. I have long had the practice of filling the 10 minutes prior to when my astronomy class starts with videos of music featuring women instrumentalists, just as I make it my practice to bring video clips of experts in the field who happen to be women into the class content. The reader may or may not be aware that the historical predicament of women in STEM fields has significant parallels to the historical predicament of women in music, particularly when it comes to women instrumentalists. Indeed, women came to be auditioned into orchestras in significant numbers only after blind auditions were introduced in the 1970s. Neither did one see women instrumentalists playing with Miles Davis, say, or the Rolling Stones. Fortunately, both pop music and STEM fields are beginning to shift in this regard. It is my hope, intent, and practice that as the younger generation comes to see women in both roles as "normal," they will help accelerate this shift. So my students hear Lari Basilio shredding on electric guitar on, say, *Alive and Living*, Sonah Jobarteh playing *Mamamuso* on the kora, and Sophie Alloway on drums with Ida Hollis on electric bass playing *Shuffle Bubble*, among many others. They likewise learn about the process of looking for life on Mars from Moogega Cooper and about the sound of black holes colliding from Janna Levin. I share all of this detail so that it will be clear why the background soundtrack to my research into the material that comprises Sections 8 and 9—and the idea that one sort of integral could act as a bridge or mathematical Rosetta stone to craft others—was guitarist, composer, and singer Sister Rosetta Tharpe. She was inducted by the Rock and Roll Hall of Fame as "the Godmother of Rock & Roll" for songs such as *Trouble In Mind*, though her influences on gospel, country, and R&B were also vast. I am a jazz drummer who has been immersed in learning these other four musical styles over the past two decades, and, thus, Sister Rosetta Tharpe has been key not only to deepening and generalizing my musical patterning but also to the joy I experience in the process. On a weekly basis, I am immersed in the creative expression of the musicians I jam with, and the rhythmical patterns they manifest in their music evoke a resonant rhythmical response in my drumming. Sometimes this response is delayed by months, because my skill level needs to grow to accommodate it. Furthermore, I sense, but cannot prove, that this response also manifests in my work as a theoretical physicist who relies heavily on pattern recognition for insights that culminate in my math-based results, such as the generalization to Equation (31) from the sequence from (28) to (30). It is with all this in mind that I dedicate this paper, and in particular the integral representations of Sections 8 and 9, to Sister Rosetta Tharpe.

Conflicts of Interest: The author declares no conflicts of interest.

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