

An integral transform for quantum amplitudes

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Abstract

The central impediment to reducing multidimensional integrals of transition amplitudes to analytic form, or at least to a fewer number of integral dimensions, is the presence of magnitudes of coordinate vector differences (square roots of polynomials) $|\mathbf{x}_1 - \mathbf{x}_2|^2 = \sqrt{x_1^2 - 2x_1x_2 \cos \theta + x_2^2}$ in disjoint products of functions. Fourier transforms circumvent this by introducing a three-dimensional momentum integral for each of those products, followed in many cases by another set of integral transforms to move all of the resulting denominators into a single quadratic form in one denominator whose square may be completed. Gaussian transforms introduce a one-dimensional integral for each such product while squaring the square roots of coordinate vector differences and moving them into an exponential. Addition theorems may also be used for this purpose, and sometimes direct integration is even possible. Each method has its strengths and weaknesses. An alternative integral transform to Fourier transforms and Gaussian transforms is derived herein and utilized. A number of consequent integrals of Macdonald functions, hypergeometric functions, and Meijer G-functions with complicated arguments is given.

Keywords: integral transform, quantum amplitudes, integrals of Macdonald functions, integrals of hypergeometric functions, integrals of Meijer G-functions

1 Introduction

The analytical reduction of atomic integrals involving explicit functions of the inter-electron distances is the central task for evaluating transition amplitudes. Direct integration is sometimes possible (see, for instance, [1], among many others), and at other times Fourier transforms (e.g. [2],[3], and [4]), Gaussian transforms (e.g., [5],[6], and [7]), and addition theorems (e.g. [8], [9], and [10]) are more useful.

The main drawback of integral transforms is that one must introduce additional integral dimensions in order to remove the initial ones, and the reduction of those introduced integrals becomes more difficult the larger the numbers of wave functions transformed. For Fourier transforms, 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 to allow the angular integrals to be performed. [11] Gaussian transforms, on the other hand, require just a single one-dimensional integral for each wave function, and the completion of the square in the coordinate variables can be done in the resulting exponential. The author nevertheless finds the former approach useful as a check on the latter.

Since more researchers are familiar with Fourier transforms, let us explicate these ideas using Gaussian transforms. Consider the a product of two Slater-type atomic orbitals, the seed function ψ_{000} from which Slater functions [12] and Hylleraas powers [4] are derived by differentiation. (Known as the Yukawa [13]

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 [14] requiring the replacement of the Coulomb potential by an effective screened potential.[15, 16] 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 $\left[R(r) = \frac{C}{\sqrt{r}}K_{1/2}(\eta r)\right]$. [17] This function also appears in the approximate ground state wave function [18] for a hydrogen atom interacting with hypothesized non-zero-mass photons.[19] For simplicity, the term *Slater orbital* will be used for this function herein.)

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

where we use the much more general notation of previous work [7] 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 j s are defined in the Gaussian transform[7] of the generalized Slater orbital:

$$\begin{aligned} V^{\eta j}(\mathbf{R}) &= R^{j-1} e^{-\eta R} = (-1)^j \frac{d^j}{d\eta^j} \frac{1}{\sqrt{\pi}} \int_0^\infty d\rho_3 \frac{e^{-R^2 \rho_3} e^{-\eta^2/4/\rho_3}}{\rho_3^{1/2}} \quad [\eta \geq 0, R > 0] \quad . \\ &= R^{j-1} e^{-\eta R} = \frac{1}{2^j \sqrt{\pi}} \int_0^\infty d\rho_3 \frac{e^{-R^2 \rho_3} e^{-\eta^2/4/\rho_3}}{\rho_3^{(j+1)/2}} H_j\left(\frac{\eta}{2\sqrt{\rho_3}}\right) \quad [\forall j \geq 0 \text{ if } \eta > 0, j = 0 \text{ if } \eta = 0] \end{aligned} \quad (2)$$

Then

$$\begin{aligned} S_1^{\eta_1 0 \eta_{12} 0}(0; 0, x_2) &= \int d^3 x_1 \frac{1}{\sqrt{\pi}} \int_0^\infty d\rho_1 \frac{e^{-x_1^2 \rho_1} e^{-\eta_1^2/4/\rho_1}}{\rho_1^{1/2}} \frac{1}{\sqrt{\pi}} \int_0^\infty d\rho_2 \frac{e^{-x_{12}^2 \rho_2} e^{-\eta_{12}^2/4/\rho_2}}{\rho_2^{1/2}} \\ &= \frac{1}{\pi} \int d^3 x'_1 \int_0^\infty d\rho_1 \frac{e^{-\eta_1^2/4/\rho_1}}{\rho_1^{1/2}} \int_0^\infty d\rho_2 \frac{e^{-\eta_{12}^2/4/\rho_2}}{\rho_2^{1/2}} \\ &\quad \times \exp\left(-(\rho_1 + \rho_2) x_1'^2 - \frac{x_2^2 \rho_1 \rho_2}{\rho_1 + \rho_2}\right), \end{aligned} \quad (3)$$

where we have not displayed the steps involved in completing the square in the quadratic form in the integration variable x_1 , which allows the spatial integral to be done by changing variables from \mathbf{x}_1 to $\mathbf{x}'_1 = \mathbf{x}_1 - \frac{\rho_2}{\rho_1 + \rho_2} \mathbf{x}_2$ with unit Jacobian,[20]

$$\int e^{-(\rho_1 + \rho_2) x_1'^2} d^3 x'_1 = 4\pi \int_0^\infty e^{-(\rho_1 + \rho_2) x_1'^2} x_1'^2 dx'_1 = \frac{4\pi^{1+1/2}}{2^2 (\rho_1 + \rho_2)^{3/2}} \quad [\rho_1 + \rho_2 > 0] \quad . \quad (4)$$

What remains is

$$\begin{aligned} S_1^{\eta_1 0 \eta_{12} 0}(0; 0, x_2) &= \pi^{1/2} \int_0^\infty d\rho_1 \frac{e^{-\eta_1^2/4/\rho_1}}{\rho_1^{1/2}} \int_0^\infty d\rho_2 \frac{e^{-\eta_{12}^2/4/\rho_2}}{\rho_2^{1/2}} \\ &\quad \times \frac{1}{(\rho_1 + \rho_2)^{3/2}} \exp\left(-\frac{x_2^2 \rho_1 \rho_2}{\rho_1 + \rho_2}\right). \end{aligned} \quad (5)$$

Let

$$\tau_1 = \frac{\rho_1}{\rho_1 + \rho_2}, \quad (6)$$

then [21]

$$\begin{aligned}
S_1^{\eta_1^0 \eta_{12}^0}(0; 0, x_2) &= \pi^{1/2} \int_0^1 d\tau \frac{1}{\tau^{1/2}} \int_0^\infty d\rho_2 \frac{1}{\rho_2^{1/2+1}} \\
&\times \exp(-x_2^2 \tau \rho_2 - (\eta_{12}^2 \tau + \eta_1^2 (1 - \tau)) / \tau / 4 / \rho_2) \\
&= \pi^{1/2} \int_0^1 d\tau \frac{1}{\tau^{1/2}} \int_0^\infty d\rho_2 \frac{1}{\rho_2^{1/2+1}} \\
&\times \exp(-x_2^2 \tau \rho_2 - (\eta_{12}^2 \tau + \eta_1^2 (1 - \tau)) / \tau / 4 / \rho_2) \\
&= \pi^{1/2} \int_0^1 d\tau \frac{2\sqrt{\pi} e^{-x_2 \sqrt{\tau(\eta_{12}^2 - \eta_1^2) + \eta_1^2}}}{\sqrt{\tau(\eta_{12}^2 - \eta_1^2) + \eta_1^2}}. \tag{7}
\end{aligned}$$

Changing variables to

$$s = [\tau(\eta_{12}^2 - \eta_1^2) + \eta_1^2]^{1/2} \tag{8}$$

allows one to perform the indefinite integration [22]

$$\begin{aligned}
S_1^{\eta_1^0 \eta_{12}^0}(0; 0, x_2) &= 2\pi \int_{\eta_1}^{\eta_{12}} \frac{2s ds}{\eta_{12}^2 - \eta_1^2} \frac{e^{-x_2 s}}{s} \\
&= 4\pi \frac{1}{\eta_{12}^2 - \eta_1^2} \frac{e^{-x_2 s}}{-x_2} \Big|_{\eta_1}^{\eta_{12}} \\
&= \frac{4\pi (e^{-\eta_{12} x_2} - e^{-\eta_1 x_2})}{x_2 (\eta_1^2 - \eta_{12}^2)}. \tag{9}
\end{aligned}$$

In an attempt to simplify this process by bypassing the latter two changes of variable, the author was able to correct an integral tabled in Prudnikov, Brychkov, and Marichev[23] that should have read

$$\int_0^\infty \int_0^\infty \frac{1}{\sqrt{x+y}} f\left(\frac{xy}{x+y}\right) e^{-px-xy} dx dy = \frac{\sqrt{\pi}(\sqrt{p}+\sqrt{q})}{\sqrt{pq}} \int_0^\infty e^{-(\sqrt{p}+\sqrt{q})^2 t} f(t) dt. \tag{10}$$

and generalize it to a wide class of integrals [24]:

$$\begin{aligned}
R_2(n, m, \nu, a, b, c, h, j, p, q) &= \int_0^\infty \int_0^\infty \frac{1}{x^{n/2} y^{m/2} (x+y)^{\nu/2}} f\left(\frac{xy}{x+y}\right) \\
&\times e^{-\frac{a}{x} - \frac{b}{y} - cxy/(x+y) - hy/(x+y) - j/(x+y) - px - qy} dx dy. \tag{11}
\end{aligned}$$

2 Seeking a simpler transform

For several years the author has been fascinated with a little-used integral transform [25]

$$\frac{1}{r_0^{s-p_1} r_1^{p_1}} = \frac{1}{\Gamma(p_1)} \int_0^\infty \frac{\zeta_1^{p_1-1}}{(r_1 \zeta_1 + r_0)^s} dt \zeta_1 \tag{12}$$

that has a tantalizing one-fewer integrals than the Gaussian transform, while nevertheless moving the coordinate variables into a single quadratic form whose square may be completed. Its downside, of course, is that it does not apply to Slater orbitals. We can nevertheless show its utility by setting $\eta_{12} = 0$ in eq. (1) and use it (with $p_1 = 1/2$ and $s = 1$) to reduce the integral over the product of one Slater orbital and one Coulomb potential:

$$\begin{aligned}
S_1^{\eta_1 000}(0; 0, x_2) &= \int d^3 x_1 \frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-0 x_{12}}}{x_{12}} \\
&= \frac{1}{\pi} \int_0^\infty x_1^2 dx_1 e^{-\eta_1 x_1} \int_0^{2\pi} d\varphi \int_0^\pi d(\cos\theta) \int_0^\infty \frac{\zeta_1^{-1/2}}{((\zeta_1 + 1)x_1^2 - 2\zeta_1 x_2 x_1 \cos\theta + \zeta_1 x_2^2)} d\zeta_1 \\
&= 2 \int_0^\infty x_1^2 dx_1 e^{-\eta_1 x_1} \int_{-1}^1 dy \int_0^\infty \frac{\zeta_1^{-1/2}}{((\zeta_1 + 1)x_1^2 - 2\zeta_1 x_2 x_1 y + \zeta_1 x_2^2)} d\zeta_1 \\
&= 2 \int_0^\infty x_1^2 dx_1 e^{-\eta_1 x_1} \int_0^\infty \zeta_1^{-1/2} d\zeta_1 \\
&\times \frac{\log((\zeta_1 + 1)x_1^2 + 2\zeta_1 x_2 x_1 + \zeta_1 x_2^2) - \log((\zeta_1 + 1)x_1^2 - 2\zeta_1 x_2 x_1 + \zeta_1 x_2^2)}{2\zeta_1 x_1 x_2} \\
&= 2 \int da \int_0^\infty x_1^2 dx_1 e^{-\eta_1 x_1} \int_0^\infty \zeta_1^{-1/2} d\zeta_1 \\
&\times \left(\frac{1}{2x_1 x_2 (a\zeta_1 + (\zeta_1 + 1)x_1^2 + 2\zeta_1 x_2 x_1)} - \frac{1}{2x_1 x_2 (at_1 + (\zeta_1 + 1)x_1^2 - 2\zeta_1 x_2 x_1)} \right) + C \\
&= \frac{4\pi(1 - e^{-\eta_1 x_2})}{x_2 \eta_1^2} + C \quad , \tag{13}
\end{aligned}$$

where we had to “renormalize” [26] this infinite logarithmic integral by taking its derivative with respect to $a = x_2^2$, whereupon integration over t was possible followed by a and then x_1 . In the ζ_1 integral, if we set $x_2 \rightarrow \infty$ the integral goes to zero. But this is also true in the last line above only if $C = 0$, giving the correct limit of eq. (9). We see in this sequence that a simpler integral-transform does not necessarily lead to an easier flow. But one can hope for both. In addition, the main failing of this integral transform is that it does not seem to be generalizable to Slater orbitals and, hence, is of lesser value.

In an exploration of alternatives, one notes that there are also several other integral transforms that might take the place of the Fourier approach and involve one-dimensional integrals rather than three per wave function. Consider for example application of [27]

$$\frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_{12} x_{12}}}{x_{12}} = \int_0^\infty \int_0^\infty \frac{2 \cos(t_1 \eta_1)}{\pi (t_1^2 + x_1^2)} \frac{2 \cos(t_2 \eta_{12})}{\pi (t_2^2 + x_{12}^2)} dt_1 dt_2 \tag{14}$$

to the initial problem.

We may again use eq. (12) (with $p_1 = 1$ and $s = 2$) to move both denominators into a common quadratic form

$$\frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_{12} x_{12}}}{x_{12}} = \frac{4}{\pi^2} \int_0^\infty \int_0^\infty \cos(t_1 \eta_1) \cos(t_2 \eta_{12}) \int_0^\infty \frac{\zeta_1^{1-1}}{(\zeta_1 (t_1^2 + x_1^2) + (t_2^2 + x_{12}^2))} d\zeta_1 dt_1 dt_2 \tag{15}$$

As the author was acknowledging that this was no improvement on the Gaussian Transform, a creative flash led to the following question: “What happens if instead of completing the square in the coordinate variables and integrating, one does the t integrals first?” The t_2 integral is just [27] again so that, [28]

$$\begin{aligned}
\frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_{12} x_{12}}}{x_{12}} &= \frac{2}{\pi} \int_0^\infty \int_0^\infty \cos(t_1 \eta_1) \frac{2}{\pi} \sqrt{\pi} 2^{-3/2} \eta_{12}^{3/2} \frac{K_{\frac{3}{2}} \left(\eta_{12} \sqrt{x_{12}^2 + (t_1^2 + x_1^2) \zeta_1} \right)}{\left(\sqrt{x_{12}^2 + (t_1^2 + x_1^2) \zeta_1} \right)^{3/2}} d\zeta_1 dt_1 \\
&= \int_0^\infty \frac{\sqrt{\zeta_1 \eta_{12}^2 + \eta_1^2} K_1 \left(\sqrt{x_1^2 + \frac{x_{12}^2}{\zeta_1}} \sqrt{\eta_1^2 + \zeta_1 \eta_{12}^2} \right)}{\pi \zeta_1^{3/2} \sqrt{x_1^2 + \frac{x_{12}^2}{\zeta_1}}} d\zeta_1 \quad . \tag{16}
\end{aligned}$$

This result is nothing less than the desired integral transform to take the place of eq. (12) for the case of two Slater orbitals. We will see that the fact that the quadratic form $x_1^2 + \frac{x_2^2}{\zeta_1}$ appears in two places is not an impediment. One simply completes the square and copies the result from one quadratic form to its identical mate. So this may indeed be simpler than the Gaussian transform for some problems.

Having the desired integral transform in hand, let us apply it to the original problem. We first complete the square in the quadratic form (changing variables from \mathbf{x}_1 to $\mathbf{x}'_1 = \mathbf{x}_1 - \frac{1}{\zeta_1+1}\mathbf{x}_2$ with unit Jacobian) so that [29, 22]

$$\begin{aligned}
S_1^{\eta_1^0 \eta_{12}^0}(0; 0, x_2) &= \int d^3 x_1 \int_0^\infty \frac{\sqrt{\zeta_1 \eta_{12}^2 + \eta_1^2} K_1 \left(\sqrt{x_1^2 + \frac{x_2^2}{\zeta_1}} \sqrt{\eta_1^2 + \zeta_1 \eta_{12}^2} \right)}{\pi \zeta_1^{3/2} \sqrt{\frac{x_2^2}{\zeta_1} + x_1^2}} d\zeta_1 \\
&= \int d^3 x'_1 \int_0^\infty \frac{\sqrt{\zeta_1 \eta_{12}^2 + \eta_1^2} K_1 \left(\sqrt{\frac{x_1'^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2}{\zeta_1 + 1}} \sqrt{\eta_1^2 + \zeta_1 \eta_{12}^2} \right)}{\pi \zeta_1^{3/2} \sqrt{\frac{x_1'^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2}{\zeta_1 + 1}}} d\zeta_1 \\
&= \int_0^\infty \frac{2\pi e^{-\frac{x_2 \sqrt{\zeta_1 \eta_{12}^2 + \eta_1^2}}{\sqrt{\zeta_1 + 1}}}}{(\zeta_1 + 1)^{3/2} \sqrt{\zeta_1 \eta_{12}^2 + \eta_1^2}} d\zeta_1 = \int_{x_2 \eta_1}^{x_2 \eta_{12}} \frac{4\pi e^{-y}}{x_2 (\eta_{12}^2 - \eta_1^2)} dy \\
&= \frac{4\pi (e^{-\eta_{12} x_2} - e^{-\eta_1 x_2})}{x_2 (\eta_1^2 - \eta_{12}^2)} , \tag{17}
\end{aligned}$$

which is indeed a much shorter path to the solution than the Gaussian and Fourier transforms give.

3 Generalization

In principle, any integral transform that converts a Slater orbital into a denominator of some power – to be combined with an integral transform like [25] – could be used for multiple products of Slater orbitals, for instance the Stieltjes Transform [30] or the Bessel function equivalent of the transform in eq. (14), [31]

$$\frac{e^{-\lambda r}}{r} = \int_0^\infty \frac{x J_0(x\lambda)}{(r^2 + x^2)^{3/2}} dx \quad . \tag{18}$$

It turns out that using the Fourier transform as this stepping stone most easily allows one to find the general form for the equivalent integral transform of eq. (16) for a product of M Slater orbitals if one takes the additional step of moving the denominator into an exponential using [32]

$$(\nu - 1)! D^{-\nu} = \int_0^\infty d\rho \rho^{\nu-1} e^{-\rho D} \quad ; \tag{19}$$

$$\begin{aligned}
\frac{e^{-R_1 \eta_1}}{R_1} \cdot \frac{e^{-R_2 \eta_2}}{R_2} \cdots \frac{e^{-R_M \eta_M}}{R_M} &= \int d^3 k_1 \int d^3 k_2 \cdots \int d^3 k_M \frac{1}{2\pi^2} \cdot \frac{e^{ik_1 \cdot R_1}}{k_1^2 + \eta_1^2} \cdot \frac{1}{2\pi^2} \cdot \frac{e^{ik_2 \cdot R_2}}{k_2^2 + \eta_2^2} \cdots \frac{1}{2\pi^2} \cdot \frac{e^{ik_M \cdot R_M}}{k_M^2 + \eta_M^2} \\
&= \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \cdots \int_0^\infty d\zeta_{M-1} \int d^3 k_1 \int d^3 k_2 \cdots \int d^3 k_M \\
&\times \frac{(M-1)! \exp(ik_1 \cdot R_1 + ik_2 \cdot R_2 + \cdots + ik_{M-1} \cdot x_{M-1} + ik_M \cdot R_M)}{16\pi^8 ((k_1^2 + \eta_1^2) + \zeta_1 (k_2^2 + \eta_2^2) + \zeta_2 (k_3^2 + \eta_{13}^2) + \cdots + \zeta_{M-1} (k_M^2 + \eta_M^2))^M} \\
&= \frac{1}{2^M \pi^{2M}} \int_0^\infty d\rho \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \cdots \int_0^\infty d\zeta_{M-1} \int d^3 k_1 \int d^3 k_2 \cdots \int d^3 k_M \\
&\times \exp(-\rho (ik_1 \cdot R_1 / \rho - ik_2 \cdot R_2 / \rho - \cdots - ik_{M-1} \cdot x_{M-1} / \rho - ik_M \cdot R_M / \rho)) \\
&\times \rho^{M-1} \exp(-\rho ((k_1^2 + \eta_1^2) + \zeta_1 (k_2^2 + \eta_2^2) + \zeta_2 (k_3^2 + \eta_{13}^2) + \cdots + \zeta_{M-1} (k_M^2 + \eta_M^2))) \\
&= \frac{1}{2^M \pi^{2M}} \int_0^\infty d\rho \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \cdots \int_0^\infty d\zeta_{M-1} \int d^3 k_1 \int d^3 k_2 \cdots \int d^3 k_M \exp(-\rho Q) \quad . \tag{20}
\end{aligned}$$

The quadratic form may be written as [11]

$$Q = \underline{V}^T \underline{W} \underline{V} \quad (21)$$

where

$$\underline{V}^T = (\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_M, 1) \quad , \quad (22)$$

$$\underline{W} = \begin{pmatrix} 1 & 0 & \cdots & 0 & \mathbf{b}_1 \\ 0 & \zeta_1 & \cdots & 0 & \mathbf{b}_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \zeta_{M-1} & \mathbf{b}_M \\ \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_M & C \end{pmatrix} \quad , \quad (23)$$

$$C = \eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \cdots + \zeta_{M-1} \eta_M^2 \quad , \quad (24)$$

and

$$\mathbf{b}_j = -\frac{i}{2\rho} \mathbf{R}_j \quad . \quad (25)$$

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

$$Q' = a'_1 k_1^2 + a'_2 k_2^2 + \dots + a'_{N+M} k_{N+M}^2 + c' \quad (26)$$

where, as shown by Chisholm, [33] the a' are positive. Then after a simple translation in $\{\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_M\}$ space (with Jacobian = 1), the k integrals could be done,[20]

$$\int d^3 k'_1 \dots d^3 k'_M e^{-\rho(a'_1 k_1'^2 + a'_2 k_2'^2 + \dots + a'_M k_M'^2)} = \left(\frac{\pi^M}{\rho^M \Lambda} \right)^{3/2} \quad , \quad (27)$$

leaving just the exponential of $-\rho c'$ to integrate over ρ and the ζ_i . But Λ is an invariant determinant

$$\Lambda = \begin{vmatrix} 1 & 0 & \cdots & 0 \\ 0 & \zeta_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \zeta_{M-1} \end{vmatrix} = (1) \prod_{i=1}^{M-1} \zeta_i = \prod_{i=1}^M a'_i \quad , \quad (28)$$

so actually finding the orthogonal transformation that reduces Q to diagonal form is unnecessary.

This orthogonal transformation also leaves

$$\Omega = \det \mathbf{W} \quad (29)$$

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

$$c' \Lambda = \Omega = C \Lambda + \sum_{i=1}^M \sum_{j=1}^M \mathbf{b}_i \cdot \mathbf{b}_j (-1)^{i+j+1} \Lambda_{ij} = C \Lambda - b_1^2 (1) \prod_{i=1}^{M-1} \zeta_i - \sum_{j=2}^M b_j^2 \prod_{i \neq j-1}^{M-1} \zeta_i \quad (30)$$

where Λ_{ij} is Λ with the i th row and j th column deleted, and this is diagonal in the present case. Therefore c' (of eq. (26)) is given by

$$\begin{aligned} c' = \Omega / \Lambda &= \eta_1^2 + \sum_{j=2}^M \zeta_{j-1} \eta_j^2 - b_1^2 - \sum_{j=2}^M b_j^2 \frac{1}{\zeta_{j-1}} \\ &= \eta_1^2 + \sum_{j=2}^M \zeta_{j-1} \eta_j^2 + \frac{R_1^2}{4\rho^2} + \sum_{j=2}^M \frac{R_j^2}{4\rho^2 \zeta_{j-1}} \end{aligned} \quad (31)$$

so that

$$\begin{aligned}
\frac{e^{-R_1 \eta_1}}{R_1} \cdot \frac{e^{-R_2 \eta_2}}{R_2} \dots \frac{e^{-R_M \eta_M}}{R_M} &= \frac{1}{2^M \pi^{2M}} \int_0^\infty d\rho \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \dots \int_0^\infty d\zeta_{M-1} \frac{\pi^{3M/2}}{\rho^{M/2+1} \prod_{i=1}^{M-1} \zeta_i^{3/2}} \\
&\times \exp\left(-\rho \left(\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \dots + \zeta_{M-1} \eta_M^2\right)\right) \\
&\times \exp\left(-\left(R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \dots + \frac{R_M^2}{\zeta_{M-1}}\right) \frac{1}{4\rho}\right) .
\end{aligned} \tag{32}$$

We perform the ρ integral [21] to give the most compact, final form for this integral transform:

$$\begin{aligned}
\frac{e^{-R_1 \eta_1}}{R_1} \cdot \frac{e^{-R_2 \eta_2}}{R_2} \dots \frac{e^{-R_M \eta_M}}{R_M} &= \frac{1}{2^M \pi^{2M}} \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \dots \int_0^\infty d\zeta_{M-1} \frac{\pi^{3M/2}}{\prod_{i=1}^{M-1} \zeta_i^{3/2}} 2^{\frac{M}{2}+1} \\
&\times \left(R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \dots + \frac{R_M^2}{\zeta_{M-1}}\right)^{-M/4} \left(\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \dots + \zeta_{M-1} \eta_M^2\right)^{M/4} \\
&\times K_{\frac{M}{2}} \left(\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \dots + \frac{R_M^2}{\zeta_{M-1}}} \sqrt{\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \dots + \zeta_{M-1} \eta_M^2}\right) .
\end{aligned} \tag{33}$$

There may be some problems for which having the inverse integration variables associated with the η 's rather than the coordinate variables would be desirable. A simple change of variables to $\zeta_i = \frac{1}{\xi_i}$ accomplishes this:

$$\begin{aligned}
\frac{e^{-R_1 \eta_1}}{R_1} \cdot \frac{e^{-R_2 \eta_2}}{R_2} \dots \frac{e^{-R_M \eta_M}}{R_M} &= \frac{1}{2^M \pi^{2M}} \int_0^\infty d\rho \int_0^\infty d\xi_1 \int_0^\infty d\xi_2 \dots \int_0^\infty d\xi_{M-1} \frac{\pi^{3M/2}}{\rho^{M/2+1} \prod_{i=1}^{M-1} \xi_i^{1/2}} \\
&\times \exp\left(-\rho \left(\eta_1^2 + \frac{\eta_2^2}{\xi_1} + \frac{\eta_3^2}{\xi_2} + \frac{\eta_4^2}{\xi_3} + \dots + \frac{\eta_M^2}{\xi_{M-1}}\right)\right) \\
&\times \exp\left(-\left(R_1^2 + \xi_1 R_2^2 + \xi_2 R_3^2 + \dots + \xi_{M-1} R_M^2\right) \frac{1}{4\rho}\right) .
\end{aligned} \tag{34}$$

$$\begin{aligned}
\frac{e^{-R_1 \eta_1}}{R_1} \frac{e^{-R_2 \eta_2}}{R_2} \dots \frac{e^{-R_M \eta_M}}{R_M} &= \frac{1}{2^M \pi^{2M}} \int_0^\infty d\xi_1 \int_0^\infty d\xi_2 \dots \int_0^\infty d\xi_{M-1} \frac{\pi^{3M/2}}{\prod_{i=1}^{M-1} \xi_i^{1/2}} 2^{\frac{M}{2}+1} , \\
&\times \left(R_1^2 + \xi_1 R_2^2 + \xi_2 R_3^2 + \dots + \xi_{M-1} R_M^2\right)^{-M/4} \left(\eta_1^2 + \frac{\eta_2^2}{\xi_1} + \frac{\eta_3^2}{\xi_2} + \frac{\eta_4^2}{\xi_3} + \dots + \frac{\eta_M^2}{\xi_{M-1}}\right)^{M/4} \\
&\times K_{\frac{M}{2}} \left(\sqrt{R_1^2 + \xi_1 R_2^2 + \xi_2 R_3^2 + \dots + \xi_{M-1} R_M^2} \sqrt{\eta_1^2 + \frac{\eta_2^2}{\xi_1} + \frac{\eta_3^2}{\xi_2} + \frac{\eta_4^2}{\xi_3} + \dots + \frac{\eta_M^2}{\xi_{M-1}}}\right) .
\end{aligned} \tag{35}$$

3.1 Inclusion of plane waves and dipole interactions

Transition amplitudes containing plane waves may be easily included in this integral transform, either directly in the ρ version prior to completing the square – by utilizing orthogonal transformation that reduces the spatial-coordinate quadratic form to diagonal form, which never needs to actually be determined, followed by a simple translation in $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ space (with Jacobian = 1) – or in the more compact version simply by applying the translation in $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ space to the plane wave(s) that multiply eqs. (33) and (35).

Photoionization transition amplitudes will generally contain dipole terms $\cos(\theta)$ that may be transformed into plane waves via a transformation like [35] $\cos\theta_{12} = -x_1^{-1} x_2^{-1} \frac{\partial}{\partial Q} \Big|_{Q=0} e^{-Q \mathbf{x}_1 \cdot \mathbf{x}_2}$, giving an integro-differential transform, whose inclusion follows that for other sorts of plane waves.

3.2 Recursion

One unusual feature of this integral transform is that one may apply the recursion relationships of Macdonald functions to lower (or raise) the indices. In particular, every trio of Slater orbitals may recursively be written as an integral of a new Slater orbital since

$$\begin{aligned}
& \frac{(\zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \eta_1^2)^{3/4} K_{\frac{3}{2}} \left(\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2}} \sqrt{\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2} \right)}{\sqrt{2} \pi^{3/2} \zeta_1^{3/2} \zeta_2^{3/2} \left(\frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + R_1^2 \right)^{3/4}} \\
&= -2 \frac{\partial}{\partial b} \exp \left(-\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2}} + b \sqrt{\zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \eta_1^2} \right) \Bigg|_{b=0} \\
& \qquad \qquad \qquad \frac{2\pi \zeta_1^{3/2} \zeta_2^{3/2} \sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + b}}{2\pi \zeta_1^{3/2} \zeta_2^{3/2} \sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + b}} \Bigg|_{b=0}
\end{aligned} \tag{36}$$

In this way, one may craft additional forms of the transformation that may be of use. For instance, for a product of four Slater orbitals, one may simply apply eq. (33) to all four orbitals simultaneous, the first form, below, or do so only for the first three, reduce the integrand to a new Slater orbital using eq. (36), and then apply eq. (33) a second time to the last orbital paired with this new one, the second form, below.

$$\begin{aligned}
& \frac{e^{-R_1 \eta_1}}{R_1} \cdot \frac{e^{-R_2 \eta_2}}{R_2} \frac{e^{-R_3 \eta_3}}{R_3} \frac{e^{-R_4 \eta_4}}{R_4} = \frac{1}{2^4 \pi^8} \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \int_0^\infty d\zeta_3 \frac{\pi^6}{\zeta_1^{3/2} \zeta_2^{3/2} \zeta_3^{3/2}} 2^3 \\
& \times \left(R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \frac{R_4^2}{\zeta_3} \right)^{-1} (\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \zeta_3 \eta_4^2)^1 \\
& \times K_2 \left(\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \frac{R_4^2}{\zeta_3}} \sqrt{\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \zeta_3 \eta_4^2} \right) \\
& = -2 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \frac{1}{2\pi \zeta_1^{3/2} \zeta_2^{3/2}} \frac{1}{2^2 \pi^4} \int_0^\infty d\zeta_3 \frac{\pi^3}{\zeta_3^{3/2}} 2^2 \\
& \frac{\partial}{\partial b} \frac{\sqrt{\zeta_3 (\zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \eta_1^2) + \eta_4^2} K_1 \left(\sqrt{R_4^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + b} \sqrt{\eta_4^2 + \zeta_3 (\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2)} \right)}{\pi \zeta_3^{3/2} \sqrt{R_4^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + b}} \Bigg|_{b=0} \\
& = -2 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \frac{1}{2\pi \zeta_1^{3/2} \zeta_2^{3/2}} \frac{1}{2^2 \pi^4} \int_0^\infty d\xi_1 \frac{\pi^3}{\xi_1^{1/2}} 2^2 \\
& \frac{\partial}{\partial b} \frac{\sqrt{\frac{1}{\xi_1} \sqrt{\frac{\zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \eta_1^2}{\xi_1} + \eta_4^2}} K_1 \left(\sqrt{R_4^2 + \left(R_2^2 + \frac{R_3^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + b \right) \xi_1} \sqrt{\eta_4^2 + \frac{\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2}{\xi_1}} \right)}{\pi \sqrt{R_4^2 + \left(R_2^2 + \frac{R_3^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + b \right) \xi_1}} \Bigg|_{b=0}
\end{aligned} \tag{37}$$

One may instead apply eq. (35) to the last orbital and the new Slater orbital obtained from eq. (36), the last form above. But redistributing ξ_1 from the first square root in the Macdonald function to the second square root gives a form quite similar to the first form, above, so it offers nothing really new apart from lowering the index on the Macdonald function by one.

4 This transform may be used as a tool to generate a class of previously-untabled integrals

The compact form of this integral transform eq. (33) involves integrals over a Macdonald function with complicated arguments that are not tabled or found in the literature to the author's knowledge, so the utility of the transform may well hinge on establishing their values. This section lays out one path to that goal, comparing sequential integration over the initially fewest number of Slater orbitals that allow one to complete the square, with simultaneous integration over larger numbers of Slater orbitals. The former approach will always yield the easiest path to a solution, while comparing these two paths will provide a suite of analytical solutions to these unusual integrals. Although this introductory paper is perhaps not the place for a full exploration of this set, we will sketch out the landscape of techniques that yield solutions.

4.1 The integral $S_1^{\eta_1 0 \eta_{12} 0 \eta_2 0}(0, 0; 0, 0, 0)$

Consider the next most difficult problem from eq. (17), including a third unshifted Slater orbital and integrating over both variables, whose solution is given easily by eq. (17), and [36]

$$\begin{aligned} S_1^{\eta_1 0 \eta_{12} 0 \eta_2 0}(0, 0; 0, 0, 0) &= \int d^3 x_2 \int d^3 x_1 \frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_{12} x_{12}}}{x_{12}} \frac{e^{-\eta_2 x_2}}{x_2} . \\ &= \int_0^\infty dx_2 4\pi x_2^2 \frac{4\pi (e^{-x_2 \eta_{12}} - e^{-x_2 \eta_1}) e^{-\eta_2 x_2}}{x_2 (\eta_1^2 - \eta_{12}^2)} \frac{1}{x_2} = \frac{16\pi^2}{(\eta_1 + \eta_2)(\eta_1 + \eta_{12})(\eta_2 + \eta_{12})} \end{aligned} \quad (38)$$

4.1.1 Transforming all three Slater orbitals simultaneously

In comparison, we next take the harder road of applying the integral transform eq. (33) to all three Slater orbitals simultaneously. The integral becomes [29, 37]

$$\begin{aligned} S_1^{\eta_1 0 \eta_{12} 0 \eta_2 0}(0, 0; 0, 0, 0) &= \int d^3 x_2 \int d^3 x_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^3 x_2 \int d^3 x_1 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \\ &\quad \frac{(\zeta_1 \eta_{12}^2 + \zeta_2 \eta_{13}^2 + \eta_1^2)^{3/4} K_{\frac{3}{2}} \left(\sqrt{x_1^2 + \frac{x_{12}^2}{\zeta_1} + \frac{x_2^2}{\zeta_2}} \sqrt{\eta_1^2 + \zeta_1 \eta_{12}^2 + \zeta_2 \eta_2^2} \right)}{\sqrt{2} \pi^{3/2} \zeta_1^{3/2} \zeta_2^{3/2} \left(\frac{x_{12}^2}{\zeta_1} + \frac{x_2^2}{\zeta_2} + x_1^2 \right)^{3/4}} \\ &= \int d^3 x_2 \int d^3 x'_1 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \\ &\quad \frac{(\zeta_1 \eta_{12}^2 + \zeta_2 \eta_{13}^2 + \eta_1^2)^{3/4} K_{\frac{3}{2}} \left(\sqrt{\frac{x_1'^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2}} \sqrt{\eta_1^2 + \zeta_1 \eta_{12}^2 + \zeta_2 \eta_2^2} \right)}{\sqrt{2} \pi^{3/2} \zeta_1^{3/2} \zeta_2^{3/2} \left(\sqrt{\frac{x_1'^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2}} \right)^{3/4}} \\ &= \int_0^\infty dx_2 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \frac{8\pi x_2^2}{(\zeta_1 + 1)^{3/2} \zeta_2^{3/2}} K_0 \left(\frac{x_2 \sqrt{\zeta_1 + \zeta_2 + 1} \sqrt{\eta_1^2 + \zeta_1 \eta_{12}^2 + \zeta_2 \eta_2^2}}{\sqrt{\zeta_1 + 1} \sqrt{\zeta_2}} \right) \\ &= \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \frac{4\pi^2}{(\zeta_1 + \zeta_2 + 1)^{3/2} (\zeta_1 \eta_{12}^2 + \zeta_2 \eta_{13}^2 + \eta_1^2)^{3/2}} \\ &= \int_0^\infty d\zeta_1 \left(\frac{8\pi^2 \sqrt{\zeta_1 + 1} \eta_{13}^2}{\sqrt{\zeta_1 \eta_{12}^2 + \eta_1^2} (\zeta_1 (\eta_{13}^2 - \eta_{12}^2) - \eta_1^2 + \eta_{13}^2)^2} - \frac{16\pi^2 \eta_{13}}{(\zeta_1 (\eta_{13}^2 - \eta_{12}^2) - \eta_1^2 + \eta_{13}^2)^2} \right. \\ &\quad \left. + \frac{8\pi^2 \sqrt{\zeta_1 \eta_{12}^2 + \eta_1^2}}{\sqrt{\zeta_1 + 1} (\zeta_1 (\eta_{12}^2 - \eta_{13}^2) + \eta_1^2 - \eta_{13}^2)^2} \right) . \end{aligned} \quad (39)$$

The first and third terms of the final integral do not seem to be tabled but the computer algebra and calculus program Mathematica 7 can do these integrals,

$$\begin{aligned} \int \frac{\sqrt{a+gx}}{\sqrt{b+hx}(c+fx)^2} dx &= \frac{1}{2} \left(\frac{2\sqrt{a+gx}\sqrt{b+hx}}{(c+fx)(ch-bf)} + \frac{(bg-ah) \log((c+fx)(ah-bg)\sqrt{af-cg}\sqrt{bf-ch})}{\sqrt{af-cg}(bf-ch)^{3/2}} \right. \\ &\quad \left. + \frac{(ah-bg)}{\sqrt{af-cg}(bf-ch)^{3/2}} \right. \\ &\quad \left. \times \log(-2f(bf-ch) \left(2\sqrt{a+gx}\sqrt{b+hx}\sqrt{af-cg}\sqrt{bf-ch} + a(2bf-ch+fhx) - bcf + bfgx - 2cghx \right) \right) \end{aligned} \quad (40)$$

yielding the result of eq. (38).

4.1.2 Can one do the ζ_2 integral before the x_2 integral?

A more challenging question, and one quite useful to the utility of future work, is whether one can do the ζ_2 integral in the fourth line of (39) before the x_2 integral, to generate the third line of eq. (17) were it and the new Slater orbital $\frac{e^{-\eta_2 x_2}}{x_2}$ to be integrated over x_2 . One may rewrite the Macdonald function in terms of a Meijer G-function as [38]

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

One would like to use the one tabled integral [39] that has roughly the right form (with $\zeta_2 = x$),

$$\begin{aligned} \int_0^\infty x^{\alpha-1} (ax^2 + bx + c)^{\frac{3}{2}-\alpha} G_{0,2}^{2,0} \left(\frac{ax^2 + bx + c}{x} \middle| \nu, -\nu \right) dx \\ = \frac{\sqrt{\pi} G_{1,3}^{3,0} \left(b + 2\sqrt{a}\sqrt{c} \middle| 0, -\alpha - \nu + \frac{3}{2}, -\alpha + \nu + 3 \right)}{2a^{3/2}} . \quad (42) \\ + \frac{\sqrt{\pi} \sqrt{c} G_{1,3}^{3,0} \left(b + 2\sqrt{a}\sqrt{c} \middle| 0, -\alpha - \nu + \frac{1}{2}, -\alpha + \nu + 2 \right)}{a} \quad (43) \end{aligned}$$

but inserting $\alpha = \frac{3}{2}$ to remove the polynomial multiplying G in the integrand leaves us with the wrong power of x . One may, however, take derivatives with respect to c of the integrand and resultant, with $\nu = 1/2$ in combination with $\nu = 0$, to show that

$$\begin{aligned} \int_0^\infty \frac{K_0 \left(2\sqrt{\frac{ax^2 + bx + c}{x}} \right)}{x^{3/2}} dx &= \int_0^\infty \frac{1}{x^{3/2}} \sqrt{\pi} e^{-2\sqrt{\frac{ax^2 + bx + c}{x}}} U \left(\frac{1}{2}, 1, 4\sqrt{\frac{ax^2 + bx + c}{x}} \right) dx \\ &= \int_0^\infty \frac{1}{2x^{3/2}} G_{0,2}^{2,0} \left(\frac{ax^2 + bx + c}{x} \middle| 0, 0 \right) dx \\ &= \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{2\sqrt{c}\sqrt{2\sqrt{a}\sqrt{c}+b}} - \frac{\sqrt{\pi} G_{1,3}^{2,1} \left(b + 2\sqrt{a}\sqrt{c} \middle| -\frac{3}{2}, 0, -\frac{1}{2} \right)}{2\sqrt{c}} . \quad (44) \\ &= \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{2\sqrt{c}} \\ &\Rightarrow \frac{\pi e^{-2\left(\frac{2\sqrt{a}\sqrt{c}}{x_2\eta_2} + \frac{x_2\eta_2}{2}\right)}}{2\sqrt{c}} \end{aligned}$$

where the reduction of the Meijer G-function is from [40] and the last step

$$\sqrt{2\sqrt{a}\sqrt{c}+b} \rightarrow \frac{2\sqrt{a}\sqrt{c}}{x_2\eta_2} + \frac{x_2\eta_2}{2} \quad (45)$$

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

$$\left\{ a \rightarrow \frac{x_2^2 \eta_2^2}{4(\zeta_1 + 1)}, b \rightarrow \frac{x_2^2 \eta_2^2}{4(\zeta_1 + 1)} \left(\frac{\zeta_1 \eta_{12}^2 + \eta_1^2}{\eta_2^2} + \zeta_1 + 1 \right), c \rightarrow \frac{1}{4} x_2^2 (\zeta_1 \eta_{12}^2 + \eta_1^2) \right\} \quad (46)$$

Inserting $\frac{2\sqrt{a}\sqrt{c}}{x_2\eta_2} + \frac{x_2\eta_2}{2} \rightarrow \frac{x_2\sqrt{\zeta_1\eta_{12}^2 + \eta_1^2}}{2\sqrt{\zeta_1 + 1}} + \frac{x_2\eta_2}{2}$ indeed gives the third line of eq. (17) were it and the new Slater orbital $\frac{e^{-\eta_2 x_2}}{x_2}$ to be integrated over x_2 .

4.1.3 Can one do the ζ_2 integral before either the x_2 or x_1 integrals?

We turn next to the question of whether the third line of eq. (39) can be first integrated over ζ_2 before either of the coordinate variables to yield the second line of eq. (17) were it and the new Slater orbital $\frac{e^{-\eta_2 x_2}}{x_2}$ to be integrated over x_2 . The technique of the previous subsection runs into an immediate roadblock since

$$\begin{aligned} & \frac{(\zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2 + \eta_1^2)^{3/4}}{\zeta_2^{3/2} \left(\frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2} + \frac{x_1^2 (\zeta_1 + 1)}{\zeta_1} \right)^{3/4}} K_{\frac{3}{2}} \left(\sqrt{\frac{x_1^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2}} \sqrt{\eta_1^2 + \zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2} \right) \\ &= \frac{(\zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2 + \eta_1^2)^{3/2}}{2 \zeta_2^{3/2} \left(\left(\frac{x_1^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2} \right) (\eta_1^2 + \zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2) \right)^{3/4}} \\ &\times G_{0,2}^{2,0} \left(\frac{1}{4} \left(\frac{x_1^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2} \right) (\eta_1^2 + \zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2) \mid \frac{3}{4}, -\frac{3}{4} \right) \end{aligned} \quad (47)$$

has the additional factor $(\zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2 + \eta_1^2)^{3/2}$ that stands in the way of using derivatives of eq. (42). So we will utilize the ρ -form of the integral transform. The ζ_2 integral is straightforward, [21]

$$\begin{aligned} S_1^{\eta_1 0 \eta_{12} 0 \eta_2 0} (0, 0; 0, 0, 0) &= \int d^3 x_2 \int d^3 x_1 \frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_{12} x_{12}}}{x_{12}} \frac{e^{-\eta_2 x_2}}{x_2} \\ &= \int d^3 x_2 \int d^3 x_1 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \int_0^\infty d\rho \\ &\times \frac{1}{8\pi^{3/2} \zeta_1^{3/2} \zeta_2^{3/2} \rho^{5/2}} \exp \left(- \left(\frac{x_{12}^2}{\zeta_1} + \frac{x_2^2}{\zeta_2} + x_1^2 \right) \frac{1}{4\rho} - \rho (\zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2 + \eta_1^2) \right) \\ &= \int d^3 x_2 \int d^3 x_1 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \int_0^\infty d\rho \frac{1}{8\pi^{3/2} \zeta_1^{3/2} \zeta_2^{3/2} \rho^{5/2}} \\ &\times \exp \left(- \left(\frac{x_1^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2} \right) \frac{1}{4\rho} - \rho (\zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2 + \eta_1^2) \right) \\ &= \int d^3 x_2 \int d^3 x_1' \int_0^\infty d\zeta_1 \int_0^\infty d\rho \\ &\times \frac{1}{4\pi x_2 \zeta_1^{3/2} \rho^2} \exp \left(- \frac{x_2^2 \zeta_1 + x_1 p^2 (\zeta_1^2 + 2\zeta_1 + 1)}{4\zeta_1 (\zeta_1 + 1) \rho} - x_2 \eta_2 - \rho (\zeta_1 \eta_{12}^2 + \eta_1^2) \right) \quad (48) \end{aligned}$$

as is the next integral over ρ [21] to yield the second line of eq. (17) were it and the new Slater orbital $\frac{e^{-\eta_2 x_2}}{x_2}$ to be integrated over x_2 .

4.2 Integrating four Slater orbitals (one shifted) over three variables,

We will do one last test of our ability to integrate Macdonald functions with complicated arguments by adding a fourth unshifted Slater orbital, with the whole integrated over a third coordinate:

$$\begin{aligned}
S_1^{\eta_1 0 \eta_{12} 0 \eta_2 0 \eta_3 0} (0, 0, 0; 0, 0, 0, 0) &= \int d^3 x_3 \int d^3 x_2 \int d^3 x_1 \frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_{12} x_{12}}}{x_{12}} \frac{e^{-\eta_2 x_2}}{x_2} \frac{e^{-x_3 \eta_3}}{x_3} \\
&= S_1^{\eta_1 0 \eta_{12} 0 \eta_2 0} (0, 0; 0, 0, 0) \int d^3 x_3 \frac{e^{-\eta_3 x_3}}{x_3} \\
&= \frac{16\pi^2}{(\eta_1 + \eta_2)(\eta_1 + \eta_{12})(\eta_2 + \eta_{12})} \int_0^\infty dx_3 4\pi x_3^2 \frac{e^{-\eta_3 x_3}}{x_3} \\
&= \int_0^\infty dx_3 4\pi x_3^2 \frac{16\pi^2}{(\eta_1 + \eta_2)(\eta_1 + \eta_{12})(\eta_2 + \eta_{12})} \frac{e^{-\eta_3 x_3}}{x_3} \\
&= \frac{64\pi^3}{(\eta_1 + \eta_2)(\eta_1 + \eta_{12})(\eta_2 + \eta_{12})\eta_3^2} .
\end{aligned} \tag{49}$$

This is Harris, Frolov, and Smith's integral I (-1, -1, -1, 0, 0, -1), [26] who applied Remiddi's technique (for whom $\eta_i = 0$) [3] to simplify the arbitrary- η_i results of Fromm and Hill.[2]

4.2.1 Integrating first over the ζ_3 variable

We will do this in the most difficult order to generate new results:

$$\begin{aligned}
S_1^{\eta_1 0 \eta_{12} 0 \eta_2 0 \eta_3 0} (0, 0, 0; 0, 0, 0, 0) &= \int d^3 x_3 \int d^3 x_2 \int d^3 x_1 \frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_{12} x_{12}}}{x_{12}} \frac{e^{-\eta_2 x_2}}{x_2} \frac{e^{-x_3 \eta_3}}{x_3} \\
&= \int d^3 x_3 \int d^3 x_2 \int d^3 x_1 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \int_0^\infty d\zeta_3 \\
&\quad \left(\zeta_2 \eta_2^2 + \zeta_3 \eta_3^2 + \zeta_1 \eta_{12}^2 + \eta_1^2 \right) K_2 \left(\sqrt{x_1^2 + \frac{x_2^2}{\zeta_1} + \frac{x_2^2}{\zeta_2} + \frac{x_3^2}{\zeta_3}} \sqrt{\eta_1^2 + \zeta_2 \eta_2^2 + \zeta_3 \eta_3^2 + \zeta_1 \eta_{12}^2} \right) \\
&\quad \times \frac{2\pi^2 \zeta_1^{3/2} \zeta_2^{3/2} \zeta_3^{3/2} \left(\frac{x_2^2}{\zeta_1} + \frac{x_2^2}{\zeta_2} + \frac{x_3^2}{\zeta_3} + x_1^2 \right)}{8\pi^2 \zeta_1^{3/2} \zeta_2^{3/2}} \\
&= \int d^3 x_3 \int d^3 x_2 \int d^3 x_1 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \int_0^\infty d\zeta_3 \\
&\quad \times \left[\frac{\zeta_3^{3/2} \eta_3^4}{8\pi^2 \zeta_1^{3/2} \zeta_2^{3/2}} + \frac{\sqrt{\zeta_3} \eta_3^2 (\zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2 + \eta_1^2)}{4\pi^2 \zeta_1^{3/2} \zeta_2^{3/2}} + \frac{(\zeta_2 \eta_2^2 + \zeta_1 \eta_{12}^2 + \eta_1^2)^2}{8\pi^2 \zeta_1^{3/2} \zeta_2^{3/2} \sqrt{\zeta_3}} \right] \\
&\quad K_2 \left(2 \sqrt{\frac{x_1'^2 (\zeta_1 + 1)}{4\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1) \zeta_3 + x_3^2 (\zeta_1 + 1) \zeta_2}{4(\zeta_1 + 1) \zeta_2 \zeta_3}} \sqrt{\eta_1^2 + \zeta_2 \eta_2^2 + \zeta_3 \eta_3^2 + \zeta_1 \eta_{12}^2} \right) \\
&\quad \left(2 \left(\frac{x_1'^2 (\zeta_1 + 1)}{4\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1) \zeta_3 + x_3^2 (\zeta_1 + 1) \zeta_2}{4(\zeta_1 + 1) \zeta_2 \zeta_3} \right) (\zeta_2 \eta_2^2 + \zeta_3 \eta_3^2 + \zeta_1 \eta_{12}^2 + \eta_1^2) \right) .
\end{aligned} \tag{50}$$

After a considerable mixing of multiple derivatives with respect to c and b of the integrand and resultant of eq. (42) with various values for ν , we were able to determine that the first of the three required integrals given in square brackets in the third line above is (with $\zeta_3 = x$)

$$\begin{aligned}
& \int_0^\infty \frac{x^{3/2} K_2 \left(2\sqrt{\frac{ax^2+bx+c}{x}} \right)}{ax^2+bx+c} dx = \int_0^\infty 16\sqrt{\pi}\sqrt{x} e^{-2\sqrt{\frac{ax^2+bx+c}{x}}} U \left(\frac{5}{2}, 5, 4\sqrt{\frac{ax^2+bx+c}{x}} \right) dx \\
& = \int_0^\infty \frac{x^{3/2}}{2(ax^2+bx+c)} G_{0,2}^{2,0} \left(\frac{ax^2+bx+c}{x} \mid 1, -1 \right) dx \\
& = \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{4a^{3/2}\sqrt{2\sqrt{a}\sqrt{c}+b}} + \frac{\pi\sqrt{c}e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{2a(2\sqrt{a}\sqrt{c}+b)} + \frac{\pi\sqrt{c}e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{4a(2\sqrt{a}\sqrt{c}+b)^{3/2}} \\
& \Rightarrow e^{-x_3\eta_3} \left(\frac{\pi e^{-\frac{4\sqrt{a}\sqrt{c}}{x_3\eta_3}}}{4a^{3/2} \left(\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2} \right)} + \frac{\pi\sqrt{c}e^{-\frac{4\sqrt{a}\sqrt{c}}{x_3\eta_3}}}{2a \left(\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2} \right)^2} + \frac{\pi\sqrt{c}e^{-\frac{4\sqrt{a}\sqrt{c}}{x_3\eta_3}}}{4a \left(\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2} \right)^3} \right) . \tag{51}
\end{aligned}$$

where the last step

$$\sqrt{2\sqrt{a}\sqrt{c}+b} \rightarrow \frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2} \tag{52}$$

again holds for

$$\begin{aligned}
\{a & \rightarrow \frac{1}{4}\eta_3^2 \left(\frac{x_2^2(\zeta_1+\zeta_2+1)}{(\zeta_1+1)\zeta_2} + \frac{x_1p^2(\zeta_1+1)}{\zeta_1} \right), \\
b & \rightarrow \frac{1}{4} \left((\zeta_2\eta_2^2 + \zeta_1\eta_{12}^2 + \eta_1^2) \left(\frac{x_2^2(\zeta_1+\zeta_2+1)}{(\zeta_1+1)\zeta_2} + \frac{x_1p^2(\zeta_1+1)}{\zeta_1} \right) + x_3^2\eta_3^2 \right) \\
c & \rightarrow \frac{1}{4}x_3^2 (\zeta_2\eta_2^2 + \zeta_1\eta_{12}^2 + \eta_1^2) \} . \tag{53}
\end{aligned}$$

Likewise, for the second term in square brackets in the third line of (50) we have

$$\begin{aligned}
& \int_0^\infty \frac{\sqrt{x}}{ax^2+bx+c} K_2 \left(2\sqrt{\frac{ax^2+bx+c}{x}} \right) dx = \int_0^\infty \frac{16\sqrt{\pi}}{\sqrt{x}} e^{-2\sqrt{\frac{ax^2+bx+c}{x}}} U \left(\frac{5}{2}, 5, 4\sqrt{\frac{ax^2+bx+c}{x}} \right) dx \\
& = \int_0^\infty \frac{\sqrt{x}}{2(ax^2+bx+c)} G_{0,2}^{2,0} \left(\frac{ax^2+bx+c}{x} \mid 1, -1 \right) dx \\
& = \frac{\pi}{2\sqrt{a}(2\sqrt{a}\sqrt{c}+b)} e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}} \left(\frac{1}{2\sqrt{2\sqrt{a}\sqrt{c}+b}} + 1 \right) \\
& \Rightarrow \sqrt{\pi} \frac{1}{\sqrt{a}} \left(\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2} \right)^{-3/2} K_{\frac{3}{2}} \left(2 \left(\frac{x_3\eta_3}{2} + \frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} \right) \right) . \tag{54}
\end{aligned}$$

Thirdly, we have

$$\begin{aligned}
& \int_0^\infty \frac{1}{\sqrt{x}(ax^2+bx+c)} K_2 \left(2\sqrt{\frac{ax^2+bx+c}{x}} \right) dx = \int_0^\infty \frac{16\sqrt{\pi}}{x^{3/2}} e^{-2\sqrt{\frac{ax^2+bx+c}{x}}} U \left(\frac{5}{2}, 5, 4\sqrt{\frac{ax^2+bx+c}{x}} \right) dx \\
& = \int_0^\infty \frac{1}{2\sqrt{x}(ax^2+bx+c)} G_{0,2}^{2,0} \left(\frac{ax^2+bx+c}{x} \mid 1, -1 \right) dx \\
& = -\frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{2\sqrt{c}(2\sqrt{a}\sqrt{c}+b)} - \frac{\pi e^{-2\sqrt{2\sqrt{a}\sqrt{c}+b}}}{4\sqrt{c}(2\sqrt{a}\sqrt{c}+b)^{3/2}} \\
& \Rightarrow \frac{\pi e^{-2\left(\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2}\right)}}{2\sqrt{c} \left(\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2} \right)^2} + \frac{\pi e^{-2\left(\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2}\right)}}{4\sqrt{c} \left(\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2} \right)^3} . \tag{55}
\end{aligned}$$

We finally sum these, weighted by their coefficients, and insert

$\frac{2\sqrt{a}\sqrt{c}}{x_3\eta_3} + \frac{x_3\eta_3}{2} \rightarrow \frac{1}{2}\sqrt{\zeta_2\eta_2^2 + \zeta_1\eta_{12}^2 + \eta_1^2}\sqrt{\frac{x_2^2(\zeta_1+\zeta_2+1)}{(\zeta_1+1)\zeta_2} + \frac{x_1p^2(\zeta_1+1)}{\zeta_1} + \frac{x_3\eta_3}{2}}$. We have checked via multidimensional numerical integration that every step in this derivation yields the value given by the last line of eq. (49).

One could, of course, continue the integration process over the remaining variables. But we will stop here since the point was not doing the most difficult derivation of a well-known result, but exploring the landscape of integrals over Macdonald functions with complicated arguments that seem heretofore not to be tabled or found in the literature.

Conclusion

We have crafted an integral transformation that may find utility in the reduction of multidimensional transition amplitudes of quantum theory. In particular, the general form was found for a product of any number of Slater orbitals, whose derivatives represent hydrogenic and Hylleraas wave functions, as well as those composed of explicitly correlated exponentials of the kind introduced by Thakkar and Smith [41]. In addition to atomic and nuclear transition amplitudes, it may also find application in plasma physics, solid-state physics, negative ion physics, and problems involving a hypothesized non-zero-mass photon.

Unlike the Gaussian and Fourier transforms, it has the peculiarity of displaying the quadratic form, whose square one will wish to complete, in two locations rather than one. We have shown that this is no impediment to its use. It has the advantage over the Gaussian transform of requiring one fewer integrals to be subsequently reduced, and many fewer than the $(3(M-1) + M - 1)$ integral dimensions that the Fourier transform introduces for a product of M Slater orbitals. In cases where integrals remain, numerical integration seems to be without problems.

Its most severe downside is likely that the quadratic forms reside within a square root as the argument of a Macdonald function. By contrast, Fromm and Hill [2] were able to leverage the nicer form of the functions their Fourier transforms gave to integrate over the angular and radial variables for a product of three Slater orbitals in the three 3D integration variables with three Slater orbitals having shifted coordinates. However, the present work is motivated by the observation that Fromm and Hill's tour de force is unlikely to be extensible to higher numbers of products or dimensions. Whether or not this new approach will even approach theirs, no less exceed it, is still an open question. We have made a start herein on finding the analytical forms to a number of integrals over such Macdonald functions, but as the number of functions with shifted coordinates grows, the difficulty of doing these integrals will likely grow. It nevertheless seems a worthwhile goal to pursue.

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