An integral transform for quantum amplitudes

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October 18, 2022

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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) \(|x_1 - x_2|^2 = \sqrt{x_1^2 - 2x_1x_2 \cos \theta + x_2^2}\) 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 moments 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 \(\psi_{000}\) 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 [19] For simplicity, the term Slater
orbital will be used for this function herein.)

\[
S^{\eta_1 \eta_2^0}_1 (0; x_2) \equiv S^{\eta_1 \eta_2^0}_1 (p_1; y_1, y_2)_{p_1 \to 0, y_1 \to 0, y_2 \to x_2, j_1 \to 0, j_2 \to 0} = \int d^3 x_1 \frac{e^{-\eta_1 x_1} e^{-\eta_2^0 x_2}}{x_1 x_2}, \quad (1)
\]

where we use the much more general notation of previous work [7] in which the short-hand form for shifted
coordinates is \( x_{12} = x_1 - x_2 \), \( p_1 \) is a momentum variable within any plane wave associated with the (first)
integration variable, the \( y_1 \) are coordinates external to the integration, and the \( j \)s are defined in the Gaussian
transform [7] of the generalized Slater orbital:

\[
V^{\eta j}_R = R^{j-1} e^{-\eta R} = (-1)^j \frac{d^j}{d \eta^j} \int_0^\infty dp_3 \frac{e^{-R^2 p_3 e^{\eta^2/4 p_3}}}{\rho_3^{1/2}} \quad [\eta \geq 0, \ R > 0]
\]

Then

\[
S^{\eta_1 \eta_2^0}_1 (0; 0, x_2) = \int d^3 x_1 \frac{1}{\sqrt{\pi}} \int_0^\infty dp_1 e^{-\eta_1^2 p_1 e^{-\eta^2_1/4 p_1}} \frac{1}{\rho_1^{1/2}} \int_0^\infty dp_2 e^{-\eta_2^0 p_2 e^{-\eta^2_2/4 p_2}} \frac{1}{\rho_2^{1/2}}
\]

\[
\times \exp \left( -\frac{x_1^2 \rho_1}{\eta_1 \rho_1 + \rho_2} - \frac{x_2^2 \rho_2}{\rho_1 + \rho_2} \right), \quad (3)
\]

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 \( x_1 \) to
\( x_1' = x_1 - \frac{x_2}{\rho_1 + \rho_2} x_2 \) with unit Jacobian [20]

\[
\int e^{-(\rho_1 + \rho_2)x_1'}^2 d^3 x_1' = 4\pi \int_0^\infty e^{-(\rho_1 + \rho_2)x_1'}^2 x_1' dx_1' = \frac{4\pi^{1+1/2}}{2^2 (\rho_1 + \rho_2)^{3/2}} \quad [\rho_1 + \rho_2 > 0]. \quad (4)
\]

What remains is

\[
S^{\eta_1 \eta_2^0}_1 (0; 0, x_2) = \pi^{1/2} \int_0^\infty dp_1 \frac{e^{-\eta_1^2 p_1 e^{\eta^2_1/4 p_1}}}{\rho_1^{1/2}} \int_0^\infty dp_2 \frac{e^{-\eta_2^0 p_2 e^{\eta^2_2/4 p_2}}}{\rho_2^{1/2}}
\]

\[
\times \frac{1}{(\rho_1 + \rho_2)^{3/2}} \exp \left( -\frac{x_1^2 \rho_1}{\rho_1 + \rho_2} \right), \quad (5)
\]

Let

\[
\tau_1 = \frac{\rho_1}{\rho_1 + \rho_2},
\]

then [21]
Changing variables to

\[ s = \left[ \tau \left( \eta_1^2 - \eta_2^2 \right) + \eta_1^2 \right]^{1/2} \]

allows one to perform the indefinite integration \[22\]

\[
S_1^{\eta_1 \eta_2} (0; 0, x_2) = 2\pi \int_{\eta_1}^{\eta_1 + 2\eta_2} \frac{2s ds}{\eta_1^2 - \eta_2^2} \frac{e^{-x^2 s}}{s} = 4\pi \frac{e^{-x^2 \eta_1^2}}{\eta_1^2} - e^{-x^2 \eta_2^2} \eta_1^2 \]

\[ x_2 (\eta_1^2 - \eta_2^2) \]

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

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

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

\[
R_2 (n, m, \nu, a, b, c, h, j, p, q) = \int_0^\infty \int_0^\infty \frac{1}{x^{n/2}y^{m/2}(x+y)^{\nu/2}} f \left( \frac{xy}{x+y} \right) \times e^{-\frac{1}{2} xy/(x+y) - h y/(x+y) - j x/(x+y) - px - qy} dx dy.
\]

## 2 Seeking a simpler transform

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

\[
\frac{1}{r_0^{n_p-1}} = \frac{1}{\Gamma(p_1)} \int_0^\infty \frac{\zeta_1^{p_1-1}}{(r_1 \zeta_1 + r_0)^s} d\zeta_1
\]

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. \[14\] 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:
\[ S_{11000} (0; 0, x_2) = \int d^3x_1 e^{-\eta_1 x_1} e^{-\eta_2 x_2} x_1 x_{12} \]
\[ = \frac{1}{\pi} \int_0^\infty x_1^2 dx_1 e^{-\eta_1 x_1} \int_0^{2\pi} d\varphi \int_0^\infty d(\cos \theta) \int_0^\infty \zeta_1^{-1/2} ((\zeta_1 + 1) x_1^2 - 2\zeta_1 x_2 x_1 \cos \theta + \zeta_1 x_2^2) d\zeta_1 \]
\[ = 2 \int_0^\infty x_1^2 dx_1 e^{-\eta_1 x_1} \int_{-1}^1 dy \int_0^\infty \zeta_1^{-1/2} ((\zeta_1 + 1) x_1^2 - 2\zeta_1 x_2 x_1 y + \zeta_1 x_2^2) d\zeta_1 \]
\[ = 2 \int_0^\infty x_1^2 dx_1 e^{-\eta_1 x_1} \int_0^\infty \zeta_1^{-1/2} d\zeta_1 \]
\[ \times \log ((\zeta_1 + 1) x_1^2 + 2\zeta_1 x_2 x_1 + \zeta_1 x_2^2) - \log ((\zeta_1 + 1) x_1^2 - 2\zeta_1 x_2 x_1 + \zeta_1 x_2^2) \frac{2\zeta_1 x_1 x_2}{2} \]
\[ \times \left( \frac{1}{2 x_1 x_2 (a \zeta_1 + (\zeta_1 + 1) x_1^2 + 2\zeta_1 x_2 x_1)} - \frac{1}{2 x_1 x_2 (a t_1 + (\zeta_1 + 1) x_1^2 - 2\zeta_1 x_2 x_1)} \right) + C \]
\[ = 4\pi \left( 1 - e^{-\eta_1 x_2} \right) + C \quad , \tag{13} \]

where we had to “renormalize” \[20\] this infinite logarithmic integral by taking its derivative with respect to \( a = x_2 \), whereupon integration over \( t \) was possible followed by \( a \) and then \( x_1 \). In the \( \zeta_1 \) integral, if we set \( x_2 \to \infty \) 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 \[27\]
\[ \frac{e^{-\eta_1 x_1} e^{-\eta_2 x_2}}{x_1 x_2} = \int_0^\infty \int_0^\infty \frac{2\cos (t_1 \eta_1)}{\pi (t_1^2 + x_1^2)} \frac{2\cos (t_2 \eta_1)}{\pi (t_2^2 + x_1^2)} dt_1 dt_2 \tag{14} \]
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

\[ \frac{e^{-\eta_1 x_1} e^{-\eta_2 x_2}}{x_1 x_2} = \frac{4}{\pi^2} \int_0^\infty \int_0^\infty \cos (t_1 \eta_1) \cos (t_2 \eta_1) \int_0^\infty \zeta_1^{-1/2} \frac{1}{(\zeta_1 (t_1^2 + x_1^2) + (t_2^2 + x_1^2))^2} d\zeta_1 dt_1 dt_2 \tag{15} \]

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, \[28\]
\[ \frac{e^{-\eta_1 x_1} e^{-\eta_2 x_2}}{x_1 x_2} = \frac{2}{\pi} \int_0^\infty \int_0^\infty \cos (t_1 \eta_1) \frac{2}{\pi} \sqrt{\pi} 2^{-3/2} \eta_1^{3/2} K_2^2 \left( \eta_2 \sqrt{x_1^2 + x_2^2} + (t_1^2 + x_1^2) \zeta_1 \right) \left( \sqrt{x_1^2 + (t_1^2 + x_1^2) \zeta_1} \right)^3 d\zeta_1 dt_1 \]
\[ = \int_0^\infty \frac{\sqrt{\zeta_1 \eta_1^2 + \eta_1^2} K_1 \left( \sqrt{x_1^2 + \frac{t_1^2}{\zeta_1}} \sqrt{\eta_1^2 + \zeta_1 \eta_1^2} \right)}{\pi \zeta_1^{3/2} \sqrt{x_1^2 + \frac{t_1^2}{\zeta_1}}} d\zeta_1 . \tag{16} \]
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 \( x_1^2 + \frac{2}{\zeta_1} \) 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 \( x_1 \) to \( x_1' = x_1 - \frac{2}{\zeta_1} x_2 \) with unit Jacobian) so that \( 29, 22 \)

\[
S_{\eta_1, \eta_2, 0}^{\eta_1, \eta_2, 0} (0, 0, x_2) = \int d^3x_1 \int_0^\infty \frac{\sqrt{\zeta_1 \eta_1^2 + \eta_1^2} K_1 \left( \frac{\sqrt{x_1^2 + \frac{2}{\zeta_1} \eta_1^2}}{\sqrt{\zeta_1^2 + x_1^2}} \right)}{\pi^{3/2} \sqrt{\zeta_1^2 + x_1^2}} \frac{d\zeta_1}{\sqrt{\zeta_1^2 + x_1^2}}.
\]

\[
= \int d^3x_1 \int_0^\infty \frac{\sqrt{\zeta_1 \eta_2^2 + \eta_2^2} K_1 \left( \frac{\sqrt{x_1^2 \eta_2^2 + \eta_2^2}}{\sqrt{\zeta_1^2 + x_1^2 \eta_2^2}} \right)}{\pi^{3/2} \sqrt{\zeta_1^2 + x_1^2 \eta_2^2}} \frac{d\zeta_1}{\sqrt{\zeta_1^2 + x_1^2 \eta_2^2}} d\zeta_1.
\]

\[
= \int_0^\infty \frac{2\pi e^{-x_2 \sqrt{\eta_1^2 + \eta_2^2}}}{(\zeta_1 + 1)^{3/2} \sqrt{\zeta_1^2 + x_2^2}} d\zeta_1 = \int_{x_2 \eta_1}^{x_2 \eta_2} \frac{4\pi e^{-y}}{x_2 (\eta_2^2 - \eta_1^2)} dy.
\]

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. \( 14, 31 \)

\[
\frac{e^{-\lambda r}}{r} = \int_0^\infty \frac{x J_0(x \lambda)}{\sqrt{r^2 + x^2}} dx.
\]

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 \( 32 \)

\[
(M - 1)!D^{-\nu} = \int_0^\infty d\rho \rho^{\nu-1} e^{-\rho D}.
\]

\[
\frac{e^{-R_1 \eta_1}}{R_1} \cdot \frac{e^{-R_2 \eta_2}}{R_2} \cdots \frac{e^{-R_M \eta_M}}{R_M} = \int d^3k_1 \int d^3k_2 \cdots \int d^3k_M \left( 1 \right) \frac{e^{ik_1 \cdot R_1}}{2\pi^2} \frac{e^{ik_2 \cdot R_2}}{2\pi^2} \cdots \frac{e^{ik_M \cdot R_M}}{2\pi^2} \frac{1}{k_1^2 + \eta_1^2} \frac{1}{k_2^2 + \eta_2^2} \cdots \frac{1}{k_M^2 + \eta_M^2}.
\]

\[
= \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \cdots \int_0^\infty d\zeta_{M-1} \int d^3k_1 \int d^3k_2 \cdots \int d^3k_M \frac{\exp(ik_1 \cdot R_1 + ik_2 \cdot R_2 + \cdots + ik_M \cdot R_M)}{16\pi^3} \frac{(k_1^2 + \eta_1^2 + \zeta_1 (k_2^2 + \eta_2^2) + \cdots + \zeta_{M-1} (k_M^2 + \eta_M^2))}{(k_1^2 + \eta_1^2 + \zeta_1 (k_2^2 + \eta_2^2) + \cdots + \zeta_{M-1} (k_M^2 + \eta_M^2))^M}.
\]

\[
= \frac{1}{2M \pi^2M} \int_0^\infty d\rho \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \cdots \int_0^\infty d\zeta_{M-1} \int d^3k_1 \int d^3k_2 \cdots \int d^3k_M \exp(-\rho Q).
\]
The quadratic form may be written as [11]

\[ Q = V^T W V \]  

where

\[ V^T = (k_1, k_2, \ldots, k_M, 1), \]  

\[ W = \begin{pmatrix} 1 & 0 & \cdots & 0 & b_1 \\ 0 & \zeta_1 & \cdots & 0 & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \zeta_{M-1} & b_M \\ b_1 & b_2 & \cdots & b_M & C \end{pmatrix}, \]  

\[ C = \eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \cdots + \zeta_{M-1} \eta_M^2, \]  

and

\[ b_j = -\frac{i}{2\rho} R_j. \]  

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

\[ Q' = a_1' k_1^2 + a_2' k_2^2 + \cdots + a_{N+M}' k_{N+M}^2 + c', \]  

where, as shown by Chisholm, [33] the \( a' \) are positive. Then after a simple translation in \( \{k_1, k_2, \cdots, k_M\} \) space (with Jacobian = 1), the \( k \) integrals could be done.[20]

\[ \int d^3k_1 \cdots d^3k_M e^{-\rho(a_1' k_1^2 + a_2' k_2^2 + \cdots + a_{N+M}' k_{N+M}^2)} = \left( \frac{\pi^M}{\rho M a} \right)^{3/2}, \]  

leaving just the exponential of \(-\rho c'\) to integrate over \( \rho \) and the \( \zeta_i \). But \( \Lambda \) is an invariant determinant

\[ \Lambda = \begin{vmatrix} 1 & 0 & \cdots & 0 \\ 0 & \zeta_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \zeta_{M-1} \end{vmatrix} = (1) \prod_{i=1}^{M-1} \zeta_i = \prod_{i=1}^{M} a_i', \]  

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

This orthogonal transformation also leaves

\[ \Omega = \det W \]  

invariant and to find its value one need only expand \( \Omega \) by minors:

\[ c' \Lambda = \Omega = CA + \sum_{i=1}^{M} \sum_{j=1}^{M} b_i \cdot b_j (-1)^{i+j+1} \Lambda_{ij} = CA - b_1^2 (1) \sum_{i=1}^{M-1} \zeta_i - \sum_{j=2}^{M} b_j^2 \prod_{i \neq j-1}^{M-1} \zeta_i \]  

where \( \Lambda_{ij} \) is \( \Lambda \) with the \( i \)th row and \( j \)th column deleted, and this is diagonal in the present case. Therefore \( c' \) (of eq. [20]) is given by

\[ c' = \frac{\Omega}{\Lambda} = \eta_1^2 + \sum_{j=2}^{M} \zeta_j \eta_j^2 - b_1^2 - \sum_{j=2}^{M} b_j^2 \frac{1}{\zeta_{j-1}} \]  

\[ = \eta_1^2 + \sum_{j=2}^{M} \zeta_{j-1} \eta_j^2 + \frac{R_1^2}{4\rho^2} + \sum_{j=2}^{M} \frac{R_j^2}{4\rho^2 \zeta_{j-1}} \]  

(31)
so that

\[
\frac{e^{-R_{1,q_1}}}{R_1} \cdot \frac{e^{-R_{2,q_2}}}{R_2} \ldots \frac{e^{-R_{M,n_M}}}{R_{M}} = \frac{1}{2^{M-1} \pi^{M/2}} \int_0^\infty d\rho \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \ldots \int_0^\infty d\zeta_{M-1} \frac{\pi^{M/2}}{\rho^{M/2+1} \prod_{i=1}^{M-1} \zeta_i^{1/2}}
\]

\[
\times \exp \left( -\rho \left( \eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \cdots + \zeta_{M-1} \eta_M^2 \right) \right)
\]

\[
\times \exp \left( -\left( R_1^2 + \frac{R_1^2}{\zeta_1} + \frac{R_2^2}{\zeta_2} + \cdots + \frac{R_{M-1}^2}{\zeta_{M-1}} \right) \frac{1}{4\rho} \right).
\]

We perform the \( \rho \) integral \([21]\) to give the most compact, final form for this integral transform:

\[
\frac{e^{-R_{1,q_1}}}{R_1} \cdot \frac{e^{-R_{2,q_2}}}{R_2} \ldots \frac{e^{-R_{M,n_M}}}{R_{M}} = \frac{1}{2^{M-1} \pi^{M/2}} \int_0^\infty d\zeta \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \ldots \int_0^\infty d\zeta_{M-1} \frac{\pi^{M/2}}{\prod_{i=1}^{M-1} \zeta_i^{1/2}} 2^{M+1}
\]

\[
\times \left( \frac{R_1^2}{\zeta_1} + \frac{R_2^2}{\zeta_2} + \cdots + \frac{R_{M-1}^2}{\zeta_{M-1}} \right)^{-M/4} \left( \eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \cdots + \zeta_{M-1} \eta_M^2 \right)^{M/4}
\]

\[
\times K_{M} \left( \sqrt{\frac{R_1^2}{\zeta_1} + \frac{R_2^2}{\zeta_2} + \cdots + \frac{R_{M-1}^2}{\zeta_{M-1}}} \right).
\]

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 \( \rho \) 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 \( \{x_1, x_2, \ldots, x_N\} \) space (with Jacobian = 1) – or in the more compact version simply by applying the translation in \( \{x_1, x_2, \ldots, x_N\} \) 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 \(35\) \( \cos \theta_{12} = -x_1^{-1} x_2^{-1} \frac{\partial}{\partial Q} \big|_{Q=0} e^{-Q x_1 \cdot x_2} \), 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
$$\left(\zeta_1 \eta_1^2 + \zeta_2 \eta_2^2 + \eta_3^2\right)^{3/4} K_\frac{1}{2} \left(\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \sqrt{\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2}}\right)$$

$$\frac{\sqrt{2\pi^{3/2} \zeta_1^{3/2} \zeta_2^{3/2}}}{\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + R_4^2}}^{3/4}$$

$$= -2 \frac{\partial}{\partial b} \exp \left(-\frac{\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + b \sqrt{\zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \eta_1^2}}}{2\pi \zeta_1^{3/2} \zeta_2^{3/2} \sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + b}}\right) \bigg|_{b=0} \tag{36}$$

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 simultaneously, 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.

$$\frac{e^{-R_1 \eta_1}}{R_1} \cdot \frac{e^{-R_2 \eta_2}}{R_2} \frac{e^{-R_3 \eta_3}}{R_3} \frac{e^{-R_4 \eta_4}}{R_4} = \frac{1}{2\pi \pi^3} \int_0^\infty \! d\zeta_1 \int_0^\infty \! d\zeta_2 \int_0^\infty \! d\zeta_3 \frac{\pi^6}{\zeta_1^{3/2} \zeta_2^{3/2} \zeta_3^{3/2} 2^3} \cdot \left(R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \frac{R_4^2}{\zeta_3}\right)^{-1} \left(\eta_1^2 + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \zeta_3 \eta_4^2\right) \cdot \left(K_2 \left(\sqrt{R_1^2 + \frac{R_2^2}{\zeta_1} + \frac{R_3^2}{\zeta_2} + \frac{R_4^2}{\zeta_3}} \right) + \zeta_1 \eta_2^2 + \zeta_2 \eta_3^2 + \zeta_3 \eta_4^2\right) \bigg|_{b=0} \tag{37}$$

One may instead apply eq. (33) to the last orbital and the new Slater orbital obtained from eq. (36), the last form above. But redistributing \(\zeta_1\) 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 $S_1^{\eta_0\eta_1\eta_2\eta_0} (0,0;0,0,0)$

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]

\[
S_1^{\eta_0\eta_1\eta_2\eta_0} (0,0;0,0,0) = \int d^3x_1 \int d^3x_2 \frac{e^{-\eta_1 x_1} e^{-\eta_1 x_1} e^{-\eta_2 x_2}}{x_1 x_2 x_{12}}.
\]

(38)

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]

\[
S_1^{\eta_0\eta_1\eta_2\eta_0} (0,0;0,0,0) = \int d^3x_1 \int d^3x_2 \int d\xi_1 \int d\zeta_1 \int d\zeta_2 \\
\times \left( (\zeta_1 \eta_1^2 + \zeta_2 \eta_2^2 + \zeta_1 \eta_1^2) \right) 3/4 K_2 \left( \sqrt{x_1^2 + \zeta_1^2 \eta_1^2} + \sqrt{x_2^2 + \zeta_2^2 \eta_2^2} + \sqrt{\eta_1^2 + \eta_2^2 + \eta_1 \eta_2 + \eta_1 \eta_2} \right)
\]

(39)

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

\[
\int \frac{\sqrt{a+gx}}{\sqrt{b+hx(c+f)x^2}} \, dx = \frac{1}{2} \left( \frac{2 \sqrt{a+gx} \sqrt{b+hx}}{(c+f)x(ch-bf)} + \frac{(bg-ah) \log \left((c+f)\sqrt{a+gx}-bg \sqrt{ch} - ch\right) }{\sqrt{a+gx} - cg \sqrt{bf-ch}} \right.
\]

(40)

+ \frac{(ah-bg)}{\sqrt{a+gx} - cg \sqrt{bf-ch}}

\times \log \left( -2f(bf-ch) \left( 2\sqrt{a+gx} \sqrt{b+hx} \sqrt{a+gx} - cg \sqrt{bf-ch} + a(2bf-ch+fx) - bcf + bfgx - 2cghx \right) \right)

\]
yielding the result of eq. (38).

4.1.2 Can one do the $\zeta_2$ 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 $\zeta_2$ 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 $e^{-q_{2}x_{2}}$ to be integrated over $x_2$. One may rewrite the Macdonald function in terms of a Meijer G-function as \[ (38) \]

\[ \frac{1}{\zeta_2^{3/2}} K_0 \left( \frac{2x_2 \sqrt{\zeta_1 + \zeta_2 + 1} \eta_2 \sqrt{\zeta_1 \eta_2^2 + \eta_2^2 + \zeta_2}}{\sqrt{\zeta_1 + 1} \sqrt{\zeta_2}} \right) = \frac{1}{2} \frac{1}{\zeta_2^{3/2}} G_{0,2}^{2,0} \left( \frac{x_2^2 (\zeta_1 + \zeta_2 + 1) \eta_2^2 (\zeta_2 + \eta_2^2 + \zeta_1 \eta_2^2)}{(\zeta_1 + 1) \zeta_2} \right) \mid 0, 0 \]

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

\[ \int_0^\infty x^{\alpha - 1} (ax^2 + bx + c)^{2-\alpha} \left( \frac{ax^2 + bx + c}{x} \right)^{\nu, -\nu} dx 
\]

\[ = \frac{\sqrt{\pi} \Gamma^{3,0}_1 \left( \frac{b + 2 \sqrt{a} \sqrt{c}}{2a^{3/2}} \right)}{2 \alpha - 3} \left( \frac{\pi \Gamma^{0,1}_1 \left( \frac{b + 2 \sqrt{a} \sqrt{c}}{2 \sqrt{c}} \right)}{2 \alpha - 3}, -\alpha - 1, -\alpha - 3 \right) \]

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

\[ \int_0^\infty K_0 \left( \frac{2 \sqrt{ax^2 + bx + c}}{x^{3/2}} \right) dx = \int_0^\infty \frac{1}{x^{3/2}} \sqrt{\pi} e^{-2 \sqrt{ax^2 + bx + c}} U \left( \frac{1}{2}, 1, 4 \sqrt{ax^2 + bx + c} \right) dx \]

\[ = \int_0^\infty \frac{1}{x^{3/2}} \sqrt{\pi} e^{-2 \sqrt{ax^2 + bx + c}} U \left( \frac{1}{2}, 1, 4 \sqrt{ax^2 + bx + c} \right) dx \]

\[ = \frac{\pi e^{-2 \sqrt{2} \sqrt{a \sqrt{c + b}}}}{2 \sqrt{c} \sqrt{2 \sqrt{a \sqrt{c + b}}} - \frac{3}{2}} \left( \frac{\sqrt{\pi} \Gamma^{2,1}_1 \left( \frac{b + 2 \sqrt{a} \sqrt{c}}{2 \sqrt{c}} \right)}{2 \sqrt{c}} \right) \]

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

\[ \sqrt{2 \sqrt{a \sqrt{c + b}}} \rightarrow \frac{2 \sqrt{a} \sqrt{c}}{x_2 \eta_2} + \frac{x_2 \eta_2}{2} \]

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

\[ \begin{cases} a \rightarrow \frac{x_2 \eta_2^2}{4 (\zeta_1 + 1)}, b \rightarrow \frac{x_2 \eta_2^2}{4 (\zeta_1 + 1)} \left( \frac{\zeta_1 \eta_2^2 + \eta_2^2}{\eta_2^2} + \zeta_1 + 1 \right), c \rightarrow \frac{1}{4} \frac{x_2^2 (\zeta_1 \eta_2^2 + \eta_2^2)}{2 \eta_2^2} \end{cases} \]

(46)

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

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4.1.3 Can one do the $\zeta_2$ 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 $\zeta_2$ 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

$$\frac{(\zeta_2 \eta_2^2 + \zeta_1 \eta_1^2 + \eta_1^2)^{3/4}}{\zeta_2^{3/2} \left( \frac{x_1^2 (\zeta_1 + 2 \zeta_1 + 1)}{\zeta_1 (\zeta_1 + 1)} \right) + x_1^2 (\zeta_1 + 2 \zeta_1 + 1)}^{3/4} K_\frac{3}{2} \left( \frac{x_1^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2} \frac{\eta_1^2}{\eta_1^2 + \zeta_2^2 \eta_2^2 + \zeta_1^2 \eta_1^2} \right)$$

$$= \frac{(\zeta_2 \eta_2^2 + \zeta_1 \eta_1^2 + \eta_1^2)^{3/2}}{2 \zeta_2^{3/2} \left( \frac{x_1^2 (\zeta_1 + 2 \zeta_1 + 1)}{\zeta_1 (\zeta_1 + 1)} \right) + x_1^2 (\zeta_1 + 2 \zeta_1 + 1)}^{3/4} \left( \frac{\eta_1^2}{\eta_1^2 + \zeta_2^2 \eta_2^2 + \zeta_1^2 \eta_1^2} \right)^{3/4} \quad (47)$$

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

$$S_{\zeta_1 \eta_1 \eta_2}^{0 \eta_1 \eta_2 \eta_0} (0, 0, 0, 0, 0) = \int d^3 x_2 \int d^3 x_1 \int_0^\infty dx_1 \int_0^\infty dx_2 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \int_0^\infty d\rho \frac{1}{8\pi^{3/2} \zeta_1^{3/2} \zeta_2^{3/2} \rho^{5/2}} \exp \left( - \left( \frac{x_1^2}{\zeta_1} + \frac{x_2^2}{\zeta_2} + x_1^2 \right) \frac{1}{4\rho} - \rho \left( \zeta_2 \eta_2^2 + \zeta_1 \eta_1^2 + \eta_1^2 \right) \right)$$

$$= \int d^3 x_2 \int d^3 x_1 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \int_0^\infty d\rho \frac{1}{8\pi^{3/2} \zeta_1^{3/2} \zeta_2^{3/2} \rho^{5/2}} \exp \left( - \left( \frac{x_1^2 (\zeta_1 + 1)}{\zeta_1} + \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2} \right) \frac{1}{4\rho} - \rho \left( \zeta_2 \eta_2^2 + \zeta_1 \eta_1^2 + \eta_1^2 \right) \right)$$

$$= \int d^3 x_2 \int d^3 x_1 \int_0^\infty d\zeta_1 \int_0^\infty d\rho \frac{1}{4\pi^{3/2} \zeta_1^{3/2} \rho^{2 \rho^2} \exp \left( - \frac{x_1^2 \zeta_1 + x_1 \rho^2 (\zeta_1^2 + 2 \zeta_1 + 1)}{4\zeta_1 (\zeta_1 + 1) \rho} - x_2 \rho \left( \zeta_1 \eta_1^2 + \eta_1^2 \right) \right)$$

as is the next integral over $\rho$ [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:
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-\(\eta_i\) results of Fromm and Hill. [2]

4.2.1 Integrating first over the \(\zeta_3\) variable

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

\[
S_{1}^{\eta_1,\eta_2,\eta_3,0}(0,0,0;0,0,0,0) = \int d^3x_3 \int d^3x_2 \int d^3x_1 \frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_2 x_2}}{x_2} \frac{e^{-\eta_3 x_3}}{x_3}
= S_{1}^{\eta_1,\eta_2,\eta_3,0}(0,0,0;0,0,0) \int d^3x_3 \int d^3x_2 \int d^3x_1 \frac{e^{-\eta_1 x_1}}{x_1} \frac{e^{-\eta_2 x_2}}{x_2} \frac{e^{-\eta_3 x_3}}{x_3}
\]

\[
= \int_0^\infty dx_3 4\pi x_3 e^{-\eta_3 x_3} \int_0^\infty dx_2 4\pi x_2 e^{-\eta_2 x_2} \int_0^\infty dx_1 4\pi x_1 e^{-\eta_1 x_1}
\]

\[
= \int_0^\infty dx_3 4\pi x_3 e^{-\eta_3 x_3} \int_0^\infty dx_2 4\pi x_2 e^{-\eta_2 x_2} \int_0^\infty dx_1 4\pi x_1 e^{-\eta_1 x_1}
\]

\[
= \frac{16\pi^2}{(\eta_1 + \eta_2)(\eta_1 + \eta_2)(\eta_2 + \eta_1)} \int_0^\infty dx_3 4\pi x_3 e^{-\eta_3 x_3}
\]

\[
= \int_0^\infty dx_3 4\pi x_3 \frac{16\pi^2}{(\eta_1 + \eta_2)(\eta_1 + \eta_2)(\eta_2 + \eta_1)} e^{-\eta_3 x_3}
\]

\[
= \frac{64\pi^3}{(\eta_1 + \eta_2)(\eta_1 + \eta_2)(\eta_2 + \eta_1)) \eta_3^2}.
\]

(49)

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 \(\nu\), we were able to determine that the first of the three required integrals given in square brackets in the third line above is (with \(\zeta_3 = x\)
\[ \int_0^\infty \frac{x^{3/2} K_2 \left( 2 \sqrt{\frac{a x^2 + bx + c}{x}} \right)}{a x^2 + bx + c} \, dx = \int_0^\infty 16 \sqrt{\pi} x e^{-2 \sqrt{\frac{a x^2 + bx + c}{x}}} U \left( \frac{5}{2}, 5, 4 \sqrt{\frac{a x^2 + bx + c}{x}} \right) \, dx \]

\[ = \int_0^\infty \frac{x^{3/2}}{2 (a x^2 + bx + c)} G_{0,2}^{2,0} \left( \frac{a x^2 + bx + c}{x} \middle| 1, -1 \right) \, dx \]

\[ = \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{4 a^{3/2} \sqrt{2 \sqrt{a c + b}}} + \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{2 a (2 \sqrt{a c + b})} + \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{4 a (2 \sqrt{a c + b})} \]

\[ \Rightarrow e^{-x_3 \eta_3} \left( \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{4 a^{3/2} \sqrt{x_3 \eta_3}} \right) + \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{2 a (2 \sqrt{x_3 \eta_3} + x_3 \eta_3)} + \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{4 a (2 \sqrt{x_3 \eta_3} + x_3 \eta_3)^3} \right) \]

where the last step

\[ \sqrt{2 \sqrt{a c + b}} \rightarrow \frac{2 \sqrt{a c}}{x_3 \eta_3} + \frac{x_3 \eta_3}{2} \]

again holds for

\[ \{ a \quad \rightarrow \quad \frac{1}{4} \eta_3^2 \left( \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2} + \frac{x_1 p_1}{\zeta_1} \right), \]

\[ b \quad \rightarrow \quad \frac{1}{4} \left( \frac{\zeta_2 \eta_3^3 + \zeta_1 \eta_1^2 + \eta_1^2}{(\zeta_1 + 1) \zeta_2} \left( \frac{x_2^2 (\zeta_1 + \zeta_2 + 1)}{(\zeta_1 + 1) \zeta_2} + \frac{x_1 p_1}{\zeta_1} \right) + \frac{x_3 \eta_3^3}{2} \right) \]

\[ c \quad \rightarrow \quad \frac{1}{4} \eta_3^2 (\zeta_2 \eta_3^3 + \zeta_1 \eta_1^2 + \eta_1^2) \} \].

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

\[ \int_0^\infty \frac{\sqrt{x}}{ax^2 + bx + c} K_2 \left( 2 \sqrt{\frac{a x^2 + bx + c}{x}} \right) \, dx = \int_0^\infty 16 \sqrt{\pi} x e^{-2 \sqrt{\frac{a x^2 + bx + c}{x}}} U \left( \frac{5}{2}, 5, 4 \sqrt{\frac{a x^2 + bx + c}{x}} \right) \, dx \]

\[ = \int_0^\infty \frac{\sqrt{x}}{2 (a x^2 + bx + c)} G_{0,2}^{2,0} \left( \frac{a x^2 + bx + c}{x} \middle| 1, -1 \right) \, dx \]

\[ = \frac{\pi}{2 a (2 \sqrt{a c + b})} e^{-2 \sqrt{2 \sqrt{a c + b}}} \left( \frac{1}{2 \sqrt{2 \sqrt{a c + b}}} + 1 \right) \]

\[ \Rightarrow \sqrt{a} \left( \frac{2 \sqrt{a c}}{x_3 \eta_3} + \frac{x_3 \eta_3}{2} \right)^{3/2} K_2 \left( 2 \left( \frac{x_3 \eta_3}{2} + \frac{2 \sqrt{a c}}{x_3 \eta_3} \right) \right) \]

Thirdly, we have

\[ \int_0^\infty \frac{1}{\sqrt{x}} (a x^2 + bx + c) K_2 \left( 2 \sqrt{\frac{a x^2 + bx + c}{x}} \right) \, dx = \int_0^\infty 16 \sqrt{\pi} x e^{-2 \sqrt{\frac{a x^2 + bx + c}{x}}} U \left( \frac{5}{2}, 5, 4 \sqrt{\frac{a x^2 + bx + c}{x}} \right) \, dx \]

\[ = \int_0^\infty \frac{1}{\sqrt{x}} (a x^2 + bx + c) G_{0,2}^{2,0} \left( \frac{a x^2 + bx + c}{x} \middle| 1, -1 \right) \, dx \]

\[ = \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{2 a (2 \sqrt{a c + b})} - \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{4 a (2 \sqrt{a c + b})^{3/2}} \]

\[ \Rightarrow \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{2 \sqrt{2 \sqrt{a c + b}}} \left( \frac{2 \sqrt{a c}}{x_3 \eta_3} + \frac{x_3 \eta_3}{2} \right)^{3/2} + \frac{\pi e^{-2 \sqrt{2 \sqrt{a c + b}}}}{4 \sqrt{2 \sqrt{a c + b}}} \left( \frac{2 \sqrt{a c}}{x_3 \eta_3} + \frac{x_3 \eta_3}{2} \right)^{3} .

(55)
We finally sum these, weighted by their coefficients, and insert
\[
\frac{2\sqrt{\xi_1\eta_1}}{x_3\eta_3} + \frac{2\eta_3}{\xi_1} \rightarrow \frac{1}{2} \sqrt{\xi_1\eta_1^2 + \xi_1\eta_2^2 + \eta_1^2} \left( \frac{x_3^2(\xi_1+\eta_1+1)}{\xi_1^2} + \frac{x_3^2(\eta_1+1)}{\xi_1} \right) + \frac{2\eta_3}{\xi_1}. \]
We have checked via multidimensional numerical integration that every step in this derivation yields the value given by the last line of eq. 19.

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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