Journal of Approximation Theory **113**, 156–163 (2001)
doi:10.1006/jath.2001.3620, available online at http://www.idealibrary.com on IDEAL®

Orthogonal Representation of Weber's Function Using Hermite Polynomials

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Communicated by Mourad Ismail

Received March 13, 2001; accepted in revised form June 14, 2001

The inner product of Weber's parabolic cylinder function and a Hermite polynomial is defined and evaluated as a new class of definite integrals, from which an orthogonal series expansion for Weber's parabolic cylinder function in terms of Hermite polynomials can then be derived.

1. INTRODUCTION AND NOTATION

Weber's parabolic cylinder functions, denoted by the symbol $D_v(x)$, stood in the theory of classical electromagnetism [3], in as much as Hermite polynomials, $H_n(x)$, provided evidence of a wave-like solution (e.g., see Merzbacher [2]) in the quantum theory of electromagnetism. Moreover, the utility of Weber's function, $D_v(x)$, in quantum mechanics and in solid-state studies of anharmonic crystals is well known in the context of a system of two coupled linear harmonic oscillators (Chapter 5.6 of Merzbacher [2]), implying that anharmonic motion in vibrationally coupled systems can be better represented by parabolic cylinder functions, rather than the usual simple-harmonic oscillator basis set, whose solution sets are well known to be described by Hermite polynomials. Implicit in the latter statement, however, and also the main impetus for inititiating the present study, is the evaluation of matrix elements, or definite integrals, of Weber's parabolic cylinder functions, which themselves are mathematically very intricate and involved, so seeking a simpler representation for the $D_v(x)$'s becomes instructive.

In particular, the representation which shall be chosen for $D_v(x)$ is an orthogonal expansion with respect to the basis set of the Hermite polynomials, whose expansion coefficients necessitate an inner product between

0021-9045/01 $35.00

the parabolic cylinder function, $D_\nu(x)$, and the Hermite polynomial, $H_n(x)$, to be evaluated. Evaluation of such an inner product has some merit in its own right, because it forms, to the author's knowledge, a useful as well as a new class of definite integrals involving the special functions, $D_\nu(x)$ and $H_n(x)$.

Let $\psi = D_\nu(x)$, with $D_\nu(x)$ as introduced above to denote Weber's parabolic cylinder function, and denote the Hermite polynomials with respect to the weight $\exp(-x^2/2)$ by $\phi = \exp(-x^2/2)\, H_n(x)$. The inner product of ψ and ϕ is then defined as the definite integral,

$$\langle \psi, \phi \rangle = \int_{-\infty}^{\infty} \exp(-\tfrac{1}{2} x^2)\, H_n(x)\, D_\nu(x)\, dx, \tag{1}$$

where ν is any real or complex number and n a nonnegative integer.

2. EVALUATION OF THE INNER PRODUCT

Multiplying the inner product (1) by $\sum_{n=0}^{\infty} t^n/n!$ and permuting the sum over the index n through the integral sign, together with the well-known generating function for Hermite's polynomial, $H_n(x)$,

$$\exp(2xt - t^2) = \sum_{n=0}^{\infty} \frac{H_n(x)\, t^n}{n!} \tag{2}$$

leads to the following modification of the integrand in Eq. (1):

$$\begin{aligned} &\sum_{n=0}^{\infty} \frac{t^n}{n!} \times \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2} x^2\right) H_n(x)\, D_\nu(x)\, dx \\ &= \int_{-\infty}^{\infty} \left(\sum_{n=0}^{\infty} \frac{H_n(x)\, t^n}{n!} \right) D_\nu(x)\, dx \\ &= \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2} x^2 + 2xt - t^2\right) D_\nu(x)\, dx. \end{aligned} \tag{3}$$

This last integral bears a similarity to a known standard form of integrals cited by Eq. 2.11.4(7) of Prudnikov *et al.* [4]:

$$\begin{aligned} &\int_{-\infty}^{\infty} \exp\left[-b(x-y)^2 + \frac{c^2x^2}{4} \right] D_\nu(cx)\, dx \\ &= \sqrt{2\pi}\, (2b)^{-(\nu+1)/2}\, (2b-c^2)^{\nu/2} \exp\left[\frac{bc^2y^2}{2(2b-c^2)} \right] D_\nu\left(\frac{cy\sqrt{2b}}{\sqrt{2b-c^2}} \right), \end{aligned} \tag{4}$$

provided the identification $b = 3/4$, $y = 4t/3$, and $c = 1$ is made, Accordingly, Eq. (3) can be evaluated to give

$$\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}x^2 + 2xt - t^2\right) D_\nu(x)\, dx = 2\sqrt{\pi}\, 3^{-\frac{(\nu+1)}{2}} \exp\left(\frac{5}{3}t^2\right) D_\nu\left(\frac{4t}{\sqrt{3}}\right). \tag{5}$$

Clearly, expanding the right hand side of Eq. (5) in powers of t^n and matching its nth-order coefficient with the corresponding nth-order coefficient on the left hand side of Eq. (3) will lead to the desired result for the inner product (1).

Starting, then, with the defining relationship between the confluent hypergeometric function, ${}_1F_1(a; c; z)$, and Weber's parabolic cylinder function, $D_\nu(x)$, (Gradshteyn and Ryhzik [1, p. 1064]),

$$D_\nu(z) = 2^{\nu/2} \exp(-z^2/4) \left[\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1-\nu}{2}\right)}\, {}_1F_1\left(-\frac{\nu}{2}; \frac{1}{2}; \frac{z^2}{2}\right) + \frac{z}{\sqrt{2}} \frac{\Gamma\left(-\frac{1}{2}\right)}{\Gamma\left(-\frac{\nu}{2}\right)}\, {}_1F_1\left(\frac{1-\nu}{2}; \frac{3}{2}; \frac{z^2}{2}\right) \right], \tag{6}$$

as well as recalling from Rainville [5, p. 23], the *Legendre's duplication formula*,

$$(\alpha)_{2n} = 2^{2n}(\alpha)_n\, (\alpha + \tfrac{1}{2})_n, \tag{7}$$

where $(\alpha)_n$ is *Pochammer's* symbol,

$$(\alpha)_n = \frac{\Gamma(\alpha + n)}{\Gamma(\alpha)}, \tag{8}$$

$\Gamma(x)$ being the gamma function, one ascertains the following power series expansion in z for each of the confluent hypergeometric functions contained in Eq. (6):

$$2^{\frac{\nu}{2}} \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1-\nu}{2}\right)} {}_1F_1\left(-\frac{\nu}{2}; \frac{1}{2}; \frac{z^2}{2}\right) \to \sum_{k=0}^{\infty} \frac{\Gamma\left(\frac{1}{2}\right) 2^{\frac{\nu}{2}-k}}{\Gamma\left(\frac{1-\nu+2k}{2}\right)} \binom{\nu}{2k} z^{2k} \tag{9}$$

$$\frac{2^{\frac{\nu}{2}} z}{\sqrt{2}} \frac{\Gamma\left(-\frac{1}{2}\right)}{\Gamma\left(-\frac{\nu}{2}\right)} {}_1F_1\left(\frac{1-\nu}{2}; \frac{3}{2}; \frac{z^2}{2}\right) \to \sum_{k=0}^{\infty} \frac{\Gamma\left(\frac{1}{2}\right) 2^{\frac{(\nu-1)}{2}-k}}{\Gamma\left(\frac{2-\nu+2k}{2}\right)} \binom{\nu}{2k+1} z^{2k+1}, \tag{10}$$

where the $\binom{x}{y}$'s represent binomial coefficients. Inserting this result into the definition for Weber's parabolic cylinder function $D_\nu(z)$, given by Eq. (6), and noting that the terms on the right hand side of (6) represent an even and an odd power series, respectively, in z, one finds that $D_\nu(z)$ can be rewritten

$$D_\nu(z) = \exp(-z^2/4) \sum_{l=0}^{\infty} \frac{\Gamma\left(\frac{1}{2}\right) 2^{\frac{(\nu-l)}{2}}}{\Gamma\left(\frac{1-\nu+l}{2}\right)} \binom{\nu}{l} z^l. \tag{11}$$

This result for $D_\nu(z)$ can be used on the right hand side of Eq. (5), together with the exponential term expanded in its usual Taylor series, to illuminate a power series expansion in the variable t,

$$\begin{aligned}
&\frac{2\sqrt{\pi}}{3^{\frac{(\nu+1)}{2}}} \exp\left(\frac{5}{3}t^2\right) D_\nu\left(\frac{4t}{\sqrt{3}}\right) \\
&= \frac{2\sqrt{\pi}}{3^{\frac{(\nu+1)}{2}}} \exp\left(\frac{1}{3}t^2\right) \sum_{l=0}^{\infty} \frac{\Gamma\left(\frac{1}{2}\right) 2^{\frac{(\nu-l)}{2}}}{\Gamma\left(\frac{1-\nu+l}{2}\right)} \binom{\nu}{l} \left(\frac{4t}{\sqrt{3}}\right)^l \\
&= \frac{2\sqrt{\pi}}{3^{\frac{(\nu+1)}{2}}} \sum_{n=0}^{\infty} \frac{t^{2n}}{3^n\, n!} \sum_{l=0}^{\infty} \frac{\Gamma\left(\frac{1}{2}\right) 2^{\frac{(\nu-l)}{2}}}{\Gamma\left(\frac{1-\nu+l}{2}\right)} \binom{\nu}{l} \left(\frac{4t}{\sqrt{3}}\right)^l \\
&= \frac{2\sqrt{\pi}}{3^{\frac{(\nu+1)}{2}}} \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} \left(\frac{4t}{\sqrt{3}}\right)^l \frac{2^{\frac{(\nu-l)}{2}} \Gamma\left(\frac{1}{2}\right)}{3^n n! \Gamma\left(\frac{1-\nu+l}{2}\right)} \binom{\nu}{l} t^{2n+l}.
\end{aligned} \tag{12}$$

By simply shifting the index m above to $m=2n+l$, and noting that $[m/2] \geqslant l \geqslant 0$, where [] is the greatest integer symbol, one can sort out the series (12) further into ascending powers of t,

$$\frac{2\sqrt{\pi}}{3^{\frac{(\nu+1)}{2}}} \sum_{m=0}^{\infty} \frac{t^m}{m!} \left(\frac{4}{\sqrt{3}}\right)^m \sum_{n=0}^{[\frac{m}{2}]} \binom{\nu}{m-2n} \frac{m!\,\Gamma\left(\frac{1}{2}\right) 2^{-4n}}{n!\,\Gamma\left(\frac{m-2n-\nu+l}{2}\right)}, \tag{13}$$

if for no apparent reason than to make a more direct comparison of the nth-order coefficient to t^n between Eqs. (3) and (13).

The required nth-order coefficient can be procured straight away from Eq. (13), so finally, the result for the inner product reads

$$\begin{aligned}\langle \psi, \phi \rangle &= \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}x^2\right) H_n(x)\, D_\nu(x)\, dx \\ &= \frac{2^{2n+1}\sqrt{\pi}}{3^{\frac{(n+\nu+1)}{2}}} \sum_{k=0}^{[\frac{n}{2}]} \binom{\nu}{n-2k} \frac{n!\,\Gamma\left(\frac{1}{2}\right) 2^{-4k}}{k!\,\Gamma\left(\frac{n-2k-\nu+1}{2}\right)}. \end{aligned} \tag{14}$$

3. ORTHOGONAL SERIES EXPANSION FOR $D_\nu(x)$

To throw a different light on the result given by Eq. (14), consider expressing the binomial coefficients in (14) in terms of Pochammer's symbols, of course using Legendre duplication formula in Eq. (7) whenever the need arises. Eq. (14), then, becomes

$$\begin{aligned}\langle \psi, \phi \rangle &= \frac{2^{2n+1}\sqrt{\pi}}{3^{\frac{(n+\nu+1)}{2}}} \frac{\Gamma(\nu+1)\,\Gamma(n+1)\,\Gamma\left(\frac{1}{2}\right)}{\Gamma(\nu-n+1)\,\Gamma\left(\frac{n-\nu+l}{2}\right)} \sum_{k=0}^{[\frac{n}{2}]} \frac{\left(\frac{-n}{2}\right)_k \left(\frac{1-n}{2}\right)_k}{\left(\frac{\nu-n+2}{2}\right)_k} \frac{(-1)^n}{2^{4n}} \\ &= \frac{2^{2n+1}\sqrt{\pi}}{3^{\frac{(n+\nu+1)}{2}}} \frac{\Gamma(\nu+1)\,\Gamma(n+1)\,\Gamma\left(\frac{1}{2}\right)}{\Gamma(\nu-n+1)\,\Gamma\left(\frac{n-\nu+l}{2}\right)} \\ &\quad \times {}_2F_1\left(\frac{-n}{2}, \frac{1-n}{2}; \frac{\nu-n+2}{2}; -\frac{1}{2^4}\right), \end{aligned} \tag{15}$$

where the hypergeometric function, ${}_2F_1(a, b; c; x)$, has been forced to reveal itself for the first time.

Assume now that Weber's parabolic cylinder function has an available orthogonal expansion, namely,

$$D_\nu(x) = \exp(-x^2/2) \sum_{k=0}^{\infty} b_k H_k(x), \tag{16}$$

where the coefficients, b_k, can be determined by multiplying (16) throughout by $\exp(-x^2/2)\, H_m(x)$ and integrating over the variable x, with the orthogonality relation for Hermite's polynomial applied, to give:

$$2^n n! \sqrt{\pi}\, b_n = \int_{-\infty}^{\infty} \exp(-x^2/2)\, H_n(x)\, D_\nu(x)\, dx. \tag{17}$$

But the integral here is just the inner product determined by Eq. (15), thereby relating the coefficients b_n with the hypergeometric function contained in Eq. (15) in the obvious way,

$$b_n = \frac{2^{(n+1)}}{3^{\frac{(n+\nu+1)}{2}}} \frac{\Gamma(\nu+1)\, \Gamma(n+1)\, \Gamma\left(\frac{1}{2}\right)}{\Gamma(\nu-n+1)\, \Gamma\left(\frac{n-\nu+l}{2}\right)} \, {}_2F_1\left(\frac{-n}{2}, \frac{1-n}{2}; \frac{\nu-n+2}{2}; -\frac{1}{2^4}\right). \tag{18}$$

Inserting this expression for the b_n's into Eq. (15) leads to the desired result,

$$D_\nu(x) = 3^{-\frac{(\nu+1)}{2}}\, \Gamma(\nu+1) \exp(-x^2/2) \sum_{n=0}^{\infty} \frac{2^{(n+1)}}{3^{\frac{(n)}{2}}} \frac{\Gamma\left(\frac{1}{2}\right) H_n(x)}{\Gamma(\nu-n+l)\, \Gamma\left(\frac{n-\nu+l}{2}\right)}$$
$$\times {}_2F_1\left(\frac{-n}{2}, \frac{1-n}{2}; \frac{\nu-n+2}{2}; -\frac{1}{2^4}\right), \tag{19}$$

for the orthogonal series expansion of $D_\nu(x)$.

4. SUMMARY

The main contribution in the present article is the evaluation of a class of integrals of the type

$$\langle \psi, \phi \rangle = \int_{-\infty}^{\infty} \exp(-\tfrac{1}{2} x^2)\, H_n(x)\, D_\nu(x)\, dx, \tag{20}$$

which defines an inner product between Weber's parabolic cylinder functions and the Hermite polynomials. As shown in Eq. (15), $\langle\psi, \phi\rangle$ can be evaluated in terms of the hypergeometric function ${}_2F_1$:

$$\langle\psi, \phi\rangle = \frac{\sqrt{\pi}\, 2^{2n+1}}{3^{\frac{(n+\nu+1)}{2}}} \frac{\Gamma(\nu+1)\,\Gamma(n+1)\,\Gamma\left(\frac{1}{2}\right)}{\Gamma(\nu-n+1)\,\Gamma\left(\frac{n-\nu+l}{2}\right)} \times {}_2F_1\left(\frac{-n}{2}, \frac{1-n}{2}; \frac{\nu-n+2}{2}; -\frac{1}{2^4}\right), \tag{21}$$

from which it followed that Weber's parabolic cylinder function, $D_\nu(x)$, can be expressed as an orthogonal series expansion in terms of the Hermite polynomials, $H_n(x)$, that is,

$$D_\nu(x) = 3^{\frac{-(\nu+1)}{2}}\,\Gamma(\nu+1)\exp\left(-\frac{1}{2}x^2\right)\sum_{n=0}^{\infty}\frac{2^{(n+1)}}{3^{\frac{(n)}{2}}}\frac{\Gamma\left(\frac{1}{2}\right)H_n(x)}{\Gamma(\nu-n+l)\,\Gamma\left(\frac{n-\nu+l}{2}\right)} \times {}_2F_1\left(\frac{-n}{2}, \frac{1-n}{2}; \frac{\nu-n+2}{2}; -\frac{1}{2^4}\right). \tag{22}$$

As pointed out in the Introduction, if future developments along the lines of solving nonlinear oscillator problems in quantum mechanics, using Weber's parabolic cylinder function as an alternative basis set, is to proceed, then the second result displayed directly above, not only provides an alternative generating function for Hermite polynomials, but also sits with a greater chance of evaluating definite integrals involving products of two or more $D_\nu(x)$'s. This is because orthogonality relations and similar properties associated with Hermite polynomials are well known and simpler to evaluate than the direct definition of Weber's parabolic cylinder function given by Gradshteyn and Ryzhik [1, p. 1064], which one can see has an awkard relation with the confluent hypergeometric function (see also Eq. (10) of the text).

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Printed in Belgium