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Generating functions for integrals of Hermite functions

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Abstract. Several known generating functions for integrals of Hermite functions are shown to be members of one class and a method for obtaining the general member of the class is devised. Some new generating functions are obtained.

1. Introduction

A generating function for integrals involving harmonic oscillator functions provides a powerful tool for evaluating such integrals, provides a means for further manipulation and, because of the convenient form of the eigenvalues of the harmonic oscillator equation, provides a means of dealing with a sum of such integrals weighted with the appropriate Boltzmann factor. In this work we provide some general results and methods for obtaining more of these generating functions and some specific results which have current applications.

The fundamental equations are the generating function for the Hermite functions,

$$\sum_{n=0}^{\infty} \frac{H_n(x)t^n}{n!} = \exp(2xt - t^2), \tag{1}$$

and the Mehler formula (Mehler 1866),

$$\sum_{n=0}^{\infty} \frac{H_n(x)H_n(y)t^n}{2^n n!} = (1-t^2)^{-1/2} \exp\{[2xt - (x^2+y^2)t^2]/(1-t^2)\}. \tag{2}$$

When $x = y$ we refer to this as the generating function for the squares of the Hermite polynomials. The normalized harmonic oscillator function we denote by,

$$\psi_m(\alpha(x+d)) = \frac{\alpha^{1/2}}{(\pi^{1/2}2^m m!)^{1/2}} \exp[-\tfrac{1}{2}\alpha^2(x+d)^2]H_m(\alpha(x+d)) = |m, \alpha, d\rangle \equiv |m\rangle. \tag{3}$$

As we have indicated we shall find it convenient to use the Dirac notation and let the scaling parameter α and displacement d be understood.

Essentially the Mehler formula itself was used by Sulzer and Wieland (1952) and by other authors since and was used for complex x and y by Birtwistle and Modinos (1972). An integration is easily performed to obtain the generating function for the overlap integral between two functions with different equilibrium distances and frequencies

(Manneback 1951). Mnatsakanyan (1971) extended the method to obtain

$$\sum_{n=0}^{\infty}\sum_{\mu=0}^{\infty} s^n t^\mu |\langle n|\mu\rangle|^2$$
$$=2\lambda[(1-s^2)(1-t^2)(1+\lambda^2)^2+4\lambda^2(s-t)^2]^{-1/2}$$
$$\times\exp\left(\frac{-2\Lambda(1-s)(1-t)}{(1+s)(1-t)+\lambda^2(1-s)(1+t)}\right) \tag{4}$$

$\lambda=(M_n\omega_n/M_\mu\omega_\mu)^{1/2}$, $\Lambda=\frac{1}{2}d^2\lambda^2$, where M_n is the reduced mass and ω_n the angular frequency of the state $|n\rangle$ and M_μ and ω_μ those of state $|\mu\rangle$. In the case when $\lambda=1$, which corresponds physically to the states having the same vibration frequency, this reduces to

$$(1-st)^{-1}\exp\left(\frac{-\Lambda(1-s)(1-t)}{1-st}\right). \tag{5}$$

Smith (1969) gives applications of results of this type and other references. A further result has been established by Mnatsakanyan and Naidis (1974) which may be written as;

$$\sum_{n,m,\lambda,\mu=0}^{\infty} a^n b^m c^\lambda d^\mu \langle n|\lambda\rangle\langle\lambda|m\rangle\langle m|\mu\rangle\langle\mu|n\rangle$$
$$=\frac{1}{1-abcd}\exp\left(\frac{-\Lambda[(1-ab)(1-cd)+(1-a)(1-b)(1-c)(1-d)]}{1-abcd}\right). \tag{6}$$

The last term in the numerator of the argument of the exponential appears with the wrong sign in Mnatsakanyan and Naidis (1974) and we have corrected it and also re-arranged the expression so as to exhibit the symmetries better. The greek letters in the expression above are understood to be associated with one set of Hermite functions and the latin letters with a second set, displaced from the first, but with the same frequency. In the limit of any of a, b, c or d becoming unity, one of the sums drops out by closure and another by orthogonality and equation (6) reduces to equation (4).

2. More general cases

It is obvious that generating functions for more involved matrix elements can be obtained and, in particular, that the result (6) can be extended to the case where the two types of state involved have different scaling.

It is possible to see that such a generating function willl have two factors, the square root which does not involve the shift distance d and an exponential term whose argument becomes more negative with increasing shift. Since integration is over $(-\infty,\infty)$ the sign of the shift is irrelevant; all the integrals are Gaussian and the argument of the exponential contains a quadratic form in d. The generating function must be invariant under the same permutations as the defining equation independently of the shift and hence the square-rooted factor and the argument of the exponential must separately be invariant under those operations of the permutation group which leave the generating function unchanged.

Equations (4), (5) and (6) are all expressions belonging to the class:

$$S_m = \sum_{n=0}^{\infty} \sum_{\text{all}\,\lambda_i=0}^{\infty} \left\langle n \left| \prod_{i=2}^{m} \right| \lambda_i \right\rangle t_i^{\lambda_i} \langle \lambda_i | t_1^n | n \rangle. \tag{7}$$

S_m is obviously finite if

$$|t_i| \leqslant 1 \qquad \text{for all } i,$$

and

$$\left| \prod_{i=1}^{m} t_i \right| < 1. \tag{8}$$

In the case that all the states $|\lambda_i\rangle$ have the same scaling factor and are referred to the same origin, then the expression reduces to a geometrical series by orthogonality and becomes

$$S_m = \left(1 - \prod_{i=1}^{m} t_i\right)^{-1}. \tag{9}$$

Introducing a vector of variables $\boldsymbol{x}$ and its transpose $\boldsymbol{x}'$, we can evaluate equation (7) by means of (Turnbull and Aitken 1945, p 175):

$$\int_{\{-\infty\}}^{\{\infty\}} \exp(-\boldsymbol{x}'\mathbf{A}\boldsymbol{x} + \mathbf{b}'\boldsymbol{x} + c)\,\mathrm{d}\boldsymbol{x} = \pi^{m/2}|\mathbf{A}|^{-1/2} \exp(\tfrac{1}{4}\mathbf{b}'\mathbf{A}^{-1}\mathbf{b} + c). \tag{10}$$

Every real matrix decomposes uniquely into a symmetric and an antisymmetric component and the antisymmetric component contributes nothing to a quadratic form. Hence, with a general matrix $\mathbf{A}$ on the left of equation (10), it is only its symmetric component which appears on the right and it is therefore convenient to arrange that our $\mathbf{A}$ be symmetric. $\mathbf{A}$ must be positive definite for the integrals to converge and the inequalities of equation (8) guarantee this.

With the convention that

$$i+1 = 1 \qquad \text{if } i = m,$$

$$i-1 = m \qquad \text{if } i = 1;$$

from m applications of the Mehler formula (2) we find that if the elements of $\mathbf{A}$ and $\mathbf{b}$ are given by

$$a_{ii} = -\frac{1}{2}\left(\frac{\alpha_{i+1}^2(1+t_{i+1}^2)}{1-t_{i+1}^2} + \frac{\alpha_i^2(1+t_i^2)}{1-t_i^2}\right)$$

$$a_{i,i+1} = a_{i+1,i} = \frac{\alpha_{i+1}^2 t_{i+1}}{1-t_{i+1}^2},$$

all other elements of $\mathbf{A}$ are equal to zero,

$$b_i = -\left(\frac{\alpha_{i+1}^2 d_{i+1}(1-t_{i+1})}{1+t_{i+1}} + \frac{\alpha_i^2 d_i(1-t_i)}{1+t_i}\right)$$

and

$$c=\sum_{i=1}^{m}-\frac{\alpha_i^2 d_i(1-t_i)}{1+t_i} \tag{11}$$

then the S_m of equation (7) is given by equation (10) on multiplying by

$$\prod_{i=1}^{m}\alpha_i(1-t_i^2)^{1/2}. \tag{12}$$

We have, therefore, proved that a specific form can be obtained for the generating function (7) for arbitrarily large m, when all the states are referred to different origins and with different scaling parameters and we have reduced the problem of obtaining such generating functions to an algebraic one. Since we started this work we have seen that of Dubé and Herzenberg (1975), who have another approach to a similar problem.

With the equations in matrix form we gain insight into the structure of the generating function: as the inverse of $\mathbf{A}$ is adj $\mathbf{A}/|\mathbf{A}|$ we see how the same factor occurs in the multiplying factor and in the denominator of the argument of the exponential in equations (4), (5) and (6). We can make progress with integrals of the type:

$$\int_{\{-\infty\}}^{\{\infty\}}(\boldsymbol{x}'\mathbf{P}_1\boldsymbol{x})^{m_1}(\boldsymbol{x}'\mathbf{P}_2\boldsymbol{x})^{m_2}\ldots\exp(-\boldsymbol{x}'\mathbf{A}\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \tag{13}$$

(Turnbull and Aitken 1945, p 183), and this gives us the possibility of obtaining many other generating functions.

The use of equations (11) and (12) to obtain (4) and (5) is straightforward since the matrix is 2×2, but tedious, so we omit the details. The general case is more difficult. Technically speaking our matrix is sparse (although this does not manifest itself until 4×4), its inverse is dense and it is irreducible. Matrices of this type occur in the numerical analysis of self-adjoint partial differential equations where its type has become known as cyclic tridiagonal.

Algorithms have been developed for solving simultaneous linear equations with such matrices as coefficients with the minimum number of manipulations (Cuthill and Varga 1959, Evans and Atkinson 1970), and these are reviewed by Temperton (1975). The algorithms use the fact that since $\mathbf{A}$ is symmetric and positive definite it can be factored in the form

$$\mathbf{A}=\mathbf{DT'TD}, \tag{14}$$

where $\mathbf{D}$ is diagonal, $\mathbf{T}'$ is the transpose of $\mathbf{T}$ which is an upper triangular matrix with unit diagonal entries so that the determinant of $\mathbf{A}$ is the product of the diagonal entries of $\mathbf{D}^2$ and we should always be able to write the determinant of $\mathbf{A}$ as the product of two factors. The algorithms give us the right-hand side of equation (10), albeit written algorithmically.

3. Applications

The adaptation of Evans' (1971) algorithm is immediate and we omit it and just give some further results. The 'ring of three' generating function which has so far been missing from the class:

$$S_3(a,b,c)=\sum_{l,m,n=0}^{\infty} a^n b^m c^l \langle n|m\rangle\langle m|l\rangle\langle l|n\rangle$$

$$=\alpha\beta\,[\![\tfrac{1}{8}\{(\alpha^2-\beta^2)[(c^2-b^2)(1-a^2)(1-\alpha^2\beta^2)-(b^2+c^2)(1+a^2)(\alpha^2-\beta^2)]$$
$$+(\alpha^2+\beta^2)[(1-b^2c^2)(1-a^2)(1+\alpha^2\beta^2)+(1+b^2c^2)(1+a^2)(\alpha^2+\beta^2)]$$
$$-16\alpha^2\beta^2abc\}]\!]^{-1/2}\exp\Big([\![-zy\alpha^2\beta^2(1-b)(1-c)(1+a)$$
$$\times\{(1+\alpha^2)[(1+\beta^2)(1-abc)-(1-\beta^2)(b-ac)]$$
$$+(1-\alpha^2)[(1+\beta^2)(ab-c)+(1-\beta^2)(bc-a)]\}-z^2\beta^2(1-b)$$
$$\times\{\beta^2(1+b)[\alpha^2(1+a^2)(1+c^2)+\tfrac{1}{2}(1+\alpha^4)(1-a^2)(1-c^2)-4\alpha^2ac]$$
$$+\alpha^2(1-b)[(1+c^2)(1-a^2)+\alpha^2(1+a^2)(1-c^2)]\}-y^2\alpha^2(1-c)$$
$$\times\{\alpha^2(1+c)[\beta^2(1+a^2)(1+b^2)+\tfrac{1}{2}(1+\beta^4)(1-a^2)(1-b^2)-4\beta^2ab]$$
$$+\beta^2(1-c)[(1+b^2)(1-a^2)+\beta^2(1+a^2)(1-b^2)]\}]\!]$$
$$\times\{(\alpha^2-\beta^2)[(c^2-b^2)(1-a^2)(1-\alpha^2\beta^2)-(b^2+c^2)(1+a^2)(\alpha^2-\beta^2)]$$
$$+(\alpha^2+\beta^2)[(1-b^2c^2)(1-a^2)(1+\alpha^2\beta^2)+(1+b^2c^2)(1+a^2)(\alpha^2+\beta^2)]$$
$$-16\alpha^2\beta^2abc\}^{-1}\Big) \tag{15}$$

where

$$\langle n|=\langle n,1,0| \qquad \langle m|=\langle m,\alpha,y| \qquad \langle l|=\langle l,\beta,z|$$

and when the three states all have the same frequency the above generating function reduces to

$$\frac{1}{1-abc}\exp\left(\frac{-zy(1+a)(1-b)(1-c)-z^2(1-ac)(1+b)-y^2(1-ab)(1+c)}{2(1-abc)}\right). \tag{16}$$

For the generalization of equation (6) to the case of different centres and frequencies,

$S_4(a,b,c,d)$

$$=\sum_{n,m,\nu,\mu} a^n b^m c^\nu d^\mu \langle n|\nu\rangle\langle\nu|m\rangle\langle m|\mu\rangle\langle\mu|n\rangle$$
$$=4\lambda^2\{(1-\lambda^4)^2(1-a^2)(1-b^2)(1-c^2)(1-d^2)+4\lambda^2[(1+\lambda^2)^2(1-abcd)^2$$
$$-(1-\lambda^2)^2(ab-cd)^2]\}^{-1/2}\exp\Big(-\Lambda^2[(1-ab)(1+cd)+\lambda^2(1+ab)(1-cd)]$$
$$\times[2\lambda^2(1-ab)(1-cd)+(1+\lambda^4)(1-a)(1-b)(1-c)(1-d)]$$
$$\times[\![\lambda^2\{(1-\lambda^4)^2(1-a^2)(1-b^2)(1-c^2)(1-d^2)/4+\lambda^2$$
$$\times[(1+\lambda^2)^2(1-abcd)^2-(1-\lambda^2)^2(ab-cd)^2]\}]\!]^{-1}\Big). \tag{17}$$

The same convention on greek and latin summation indices holds as in equation (6) and

λ and Λ are as defined in equation (4). Equation (17) reduces to equations (4), (5) and (6) in all the appropriate limiting cases.

4. A different class of integrals

One of the most important applications of the foregoing work is in the 'compound limit' of the theory of vibrational excitation by Herzenberg and Mandl (1962). In this section we evaluate the integrals occurring in the alternative model, the 'impulse limit', and also obtain generating functions for them.

We require

$$I_{mn} = \left| \int_{-\infty}^{\infty} \frac{H_m(x)H_n(x)\exp(-x^2)}{x-c}\,\mathrm{d}x \right|^2 \tag{18}$$

where c is complex and $H_m(x)$ is the Hermite polynomial. Herzenberg and Mandl (1962) discussed approximate results for the case $m = 0$.

First consider the integrals within the moduli signs. They exist in the ordinary (Riemann) sense and we can obtain bounds on them; for example from Reuter's inequality on the Hermite functions (Reuter 1949) and the Schwarz inequality we can show that $I_{mn} < 8\pi$. We could also obtain numerical values by means of a single Gaussian quadrature. They can also be evaluated by extending into the complex plane and using the Cauchy residue theorem but we cannot simply close the contour by the familiar infinite semicircle because of the essential singularity in the integrand as $z \to \mathrm{i}R$. Simple deformations of the contour do not help and we cannot extend $\exp(-x^2)$ to $\exp(-|z|^2)$ since then the Cauchy–Riemann conditions are not satisfied. Even the Hermite functions of asymptotically large order are not of quite the right form for the application of Jordan's lemma.

The problem has been solved by Watson (Whittaker and Watson 1927, p 353), using the properties of Weber functions (parabolic cylinder functions):

$$\int_{-\infty}^{\infty} \frac{\exp(-z^2/4)D_n(z)}{z-x}\,\mathrm{d}z = \pm\mathrm{i}\sqrt{2\pi}\,\Gamma(n+1)\exp(\mp\tfrac{1}{2}n\pi\mathrm{i}-\tfrac{1}{4}x^2)D_{-n-1}(\mp\mathrm{i}x). \tag{19}$$

We have retained the notation of Whittaker and Watson so that in this formula (19) z is real, x is complex and the upper or lower sign is to be taken depending on whether the imaginary part of x is positive or negative. The factor of $\frac{1}{2}$ is missing from the exponent of the exponential in Whittaker and Watson (though this does not greatly affect our present work). A statement of the result in Erdélyi (1954, p 395) is incomplete and incorrect and equation 3 on p 288 of the same book is incomplete.

For non-negative integer n the Hermite polynomials $H_n(z)$ are related to the parabolic cylinder functions $D_n(z)$ by;

$$D_n(z) = \exp(-z^2/4)2^{-n/2}H_n(2^{-1/2}z) \tag{20}$$

and the parabolic cylinder functions of negative order are related to those of non-negative order by

$$D_n(z) = \frac{\Gamma(n+1)}{(2\pi)^{1/2}}(\mathrm{e}^{n\pi\mathrm{i}/2}D_{-n-1}(\mathrm{i}z) + \mathrm{e}^{-n\pi\mathrm{i}/2}D_{-n-1}(-\mathrm{i}z). \tag{21}$$

Watson's result can be obtained by using the above equation (21) to substitute for

$D_n(z)$, rotating the path of integration so that it runs along the imaginary axis and closing by an infinite semicircle in the left or right half-planes. The essential singularity having been avoided, the contribution from along the infinite semicircle is infinitesimal in the usual way (Whittaker and Watson 1927 give the asymptotic behaviour of the parabolic cylinder functions) and the result is obtained from the calculus of residues. Only one of the two terms from equation (21) contributes since both terms are analytic everywhere except at a single simple pole each, and these lie on opposite sides of the imaginary axis. Obviously, the result holds for $n = 0$ in addition to the positive integer n as stated by Whittaker and Watson (1927) and hence we deduce that:

$$\int_{-\infty}^{\infty} \frac{\exp(-a^2z^2-2bz)}{z-c}\,\mathrm{d}z$$
$$= \pm \mathrm{i}\sqrt{2\pi}\exp[\tfrac{1}{2}(-a^2c^2-2bc+b^2/a^2)]D_{-1}(\mp\sqrt{2}\mathrm{i}(b/a+ca)). \tag{22}$$

a and b are assumed real, c is complex and the same sign convention holds throughout as in Watson's formula. In this work n is taken to be a non-negative integer.

From (22) we are already in a position to deduce several generating functions. Substituting the generating function for the Hermite functions themselves (1) and reversing the order of integration and summation, which we can do since we have uniform convergence, we obtain for $|t|<1$,

$$\sum_{n=0}^{\infty} \frac{t^n}{n!}\int_{-\infty}^{\infty} \frac{\exp(-x^2)H_n(x)}{x-c}\,\mathrm{d}x = \pm\mathrm{i}\sqrt{2\pi}\exp[(c-t)^2/2]D_{-1}(\mp\sqrt{2}\mathrm{i}(c-t)). \tag{23}$$

The similar result, expressed entirely in terms of the parabolic cylinder functions,

$$\sum_{m=0}^{\infty} \frac{t^m}{m!}\int_{-\infty}^{\infty} \frac{\exp(-z^2/4)D_m(z)}{z-x}\,\mathrm{d}z = \pm\mathrm{i}\sqrt{2\pi}\exp[-\tfrac{1}{4}(x-t)^2]D_{-1}(\mp\mathrm{i}(x-t)), \tag{24}$$

is of interest since by differentiating n times with respect to t and using the property

$$\frac{\mathrm{d}^m}{\mathrm{d}z^m}[\exp(z^2/4)D_\nu(z)] = (-1)^m(-\nu)_m D_{\nu-m}(z) \tag{25}$$

and setting $t=0$ we recover Watson's result and thereby prove the statement before equation (22).

From the generating function for the square of the Hermite functions (2) we also obtain

$$\sum_{n=0}^{\infty} \frac{t^n}{2^n n!}\int_{-\infty}^{\infty} \frac{\exp(-x^2)H_n^2(x)}{x-c}\,\mathrm{d}x$$
$$= \pm\mathrm{i}\sqrt{2\pi}\exp\left[-\frac{c^2}{2}\left(\frac{1-t}{1+t}\right)\right]D_{-1}\left(\mp\sqrt{2}\mathrm{i}c\left(\frac{1-t}{1+t}\right)^{1/2}\right). \tag{26}$$

Using the generating function for the Hermite functions (1) twice we obtain:

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{t^n}{n!}\frac{s^m}{m!}\int_{-\infty}^{\infty} \frac{\exp(-x^2)H_n(x)H_m(x)}{x-c}\,\mathrm{d}x$$
$$= \pm\mathrm{i}\sqrt{2\pi}\exp\left(\frac{-t^2-s^2-c^2}{2}+ct+cs+st\right)D_{-1}(\mp\sqrt{2}\mathrm{i}(c-s-t)). \tag{27}$$

This result is easily generalized to obtain generating functions for integrals of this type with any number of Hermite functions in the numerator of the integrand, even when displaced and scaled as is frequently required. But we go on to consider another approach, to obtain the generating function for equation (18).

5. An alternative approach

Consider

$$\int_{-\infty}^{\infty} \frac{\exp(-x^2/4+b^x)D_{-n-1}(\mathrm{i}x)\,\mathrm{d}x}{x-c}$$
$$=(2\pi)^{3/2}(\pm\mathrm{i})\exp(-c^2/4+bc)D_n(c)\exp(\mp n\pi\mathrm{i}/2)/\Gamma(n+1). \qquad (28)$$

The proof follows the method for proving Watson's result. And consider also the integral

$$I=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\exp[-a^2(x^2+y^2)+2bxy]\,\mathrm{d}x\,\mathrm{d}y}{(x-c')(y-c)} \qquad (29)$$

where c and c' are complex and we implicitly assume that they lie on opposite sides of the real axis. The order of integration is immaterial and by Watson's result (19)

$$I=\pm\mathrm{i}\sqrt{2\pi}\int_{-\infty}^{\infty} \frac{\exp[-a^2x^2+(-a^2c^2+2bcx+b^2x^2/a^2)/2]}{x-c'}D_{-1}\left(\mp\sqrt{2}\mathrm{i}\left(-\frac{bx}{a}+ca\right)\right)\mathrm{d}x. \qquad (30)$$

Now using the result (28) with some manipulation we evaluate the integral (30) to find:

$$I=4\pi^2\exp[-a^2(c^2+c'^2)+2bcc']. \qquad (31)$$

This last result can be obtained directly from the theory of a function of two complex variables by writing

$$I=\int\int\frac{\exp[-a^2(z^2+z'^2)+2bzz']\,\mathrm{d}z\,\mathrm{d}z'}{(z-c)(z'-c')}=\pm(2\pi)^2\exp[-a^2(c^2+c'^2)+2bcc'], \qquad (32)$$

where z and z' are two independent complex variables; and integrating along closed contours which lie along the real z and z' axes and around c in the z plane and c' in the z' plane and then evaluating by residues. The result is much easier to derive using two complex variables due to the fundamental difference that by a corollary to the Riemann extension theorem, any isolated singularity of a holomorphic function of more than one complex variable is removable. Assuming, as before, that c and c' lie on opposite sides of their respective real axes gives us the result with the positive sign. If the signs of the imaginary parts of c and c' are the same the result is to be multiplied by a minus sign, since we are integrating around contours in the z and z' planes in the same sense. It is clear that the result is finite for all positive, real values of a^2 and values of $b^2 \leqslant a^4$.

By using these results we can prove directly that:

$$\int_{\mathrm{L}} \frac{\mathrm{d}x}{x-d} \int_{-\infty}^{\infty} \frac{\exp(-z^2/2+zt-t^2/2)}{z-x} \mathrm{d}z$$

$$= \sum_{n=0}^{\infty} \frac{t^n}{n!} \int_{\mathrm{L}} \frac{\mathrm{d}x}{x-d} \int_{-\infty}^{\infty} \frac{\exp(-z^2/4)D_n(z)}{z-x} \mathrm{d}z$$

$$= (2\pi)^2 \exp(-d^2/2+dt-t^2/2), \tag{33}$$

where we have used equations (1) and (20).

In other words, the parabolic cylinder functions satisfy the integral equation:

$$(2\pi)^2 \exp(-d^2/4)D_n(d) = \int_{\mathrm{L}} \frac{\mathrm{d}x}{x-d} \int_{-\infty}^{\infty} \frac{\exp(-z^2/4)D_n(z)}{z-x} \mathrm{d}z. \tag{34}$$

Here L is a contour which runs from $-\infty$ to ∞ and is deformed off the real axis into the complex plane. In the limiting case of L being the real axis then equations (33) and (34) become the Poincaré–Bertrand equation.

We also prove, using (19) and (28) or from the generating function for the parabolic cylinder functions ((1) and (20)) and (29) and (31) or by expressing the parabolic cylinder function of the sum of two variables as the sum of products of parabolic cylinder functions of the two variables and using (19) and (28), or directly from the theory of functions of two complex variables that:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\exp[-(x+y)^2/4]D_n(x+y)}{(x-c)(y-c')} \mathrm{d}x\, \mathrm{d}y = \pm(2\pi)^2 \exp[-(c+c')^2/4]D_n(c+c'). \tag{35}$$

The same sign applies as for equation (32).

6. More applications

Using equation (31) above and the Mehler formula (2) we find

$$\sum_{n=0}^{\infty} \frac{t^n}{2^n n!} \left| \int_{-\infty}^{\infty} \frac{\exp(-x^2)H_n(x)}{x-c} \mathrm{d}x \right|^2$$

$$= \frac{1}{(1-t^2)^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}y \frac{\exp\{[2xyt-(x^2+y^2)]/(1-t^2)\}}{(x-c)(y-c^*)}$$

$$= \frac{(2\pi)^2}{(1-t^2)^{1/2}} \exp\left(\frac{-(c^2+c^{*2}-2tcc^*)}{1-t^2}\right), \tag{36}$$

where c^* is the complex conjugate of c. Writing $c = \epsilon + \mathrm{i}\gamma$ the above expression equals

$$\frac{(2\pi)^2}{(1-t^2)^{1/2}} \exp\left(\frac{-2\epsilon^2}{1+t} + \frac{2\gamma^2}{1-t}\right). \tag{37}$$

The limit $\mathrm{Im}(c) = \gamma$ tends to zero is well behaved and interesting, for we recognize the generating function for the Hermite functions themselves (2):

$$\lim_{\gamma \to 0} \left| \int_{-\infty}^{\infty} \frac{\exp(-x^2)H_n(x)\,\mathrm{d}x}{x-\epsilon-\mathrm{i}\gamma} \right|^2 = \mathrm{e}^{-2\epsilon} H_n^2(\epsilon), \tag{38}$$

which is the result obtained in this limiting case by Herzenberg and Mandl (1962), who used the well known formula:

$$\lim_{\epsilon\to 0}\frac{1}{x-x_0-\mathrm{i}\epsilon}=\mathrm{P}\left(\frac{1}{x-x_0}\right)+\mathrm{i}\pi\delta(x-x_0). \tag{39}$$

The limit $\epsilon=0$ is also of interest since it gives us the maxima and in this case we recognize the generating function for

$$(2\pi)^2\exp(2\gamma^2)|H_n(\mathrm{i}\gamma x)|^2. \tag{40}$$

A qualitative discussion of this has been given by Herzenberg and Mandl (1962). We also recognize the explicit form of the moduli of the integrals:

$$\begin{aligned}\left|\int_{-\infty}^{\infty}\frac{\exp(-x^2)H_n(x)}{x-c}\,\mathrm{d}x\right|^2&\\ &=|2\pi H_n(c)\exp(-c^2)|^2\\ &=2^n(2\pi)\Gamma^2(n+1)|\exp(-c^2/2)D_{-n-1}(\mathrm{i}\sqrt{2}c)|^2.\end{aligned} \tag{41}$$

We can make this last equality by reason of the values of the integrals being known from Watson's formula (19). The case $n=0$ is of particular value:

$$D_{-1}(\mathrm{i}c)D_{-1}(-\mathrm{i}c^*)=(2\pi)^2\exp[-(c^2+c^{*2})/4]. \tag{42}$$

Using the Mehler formula (2) twice and carrying out a similar procedure we obtain the generating function:

$$\begin{aligned}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{s^mt^n}{2^{m+n}m!n!}\left|\int_{-\infty}^{\infty}\frac{H_n(x)H_m(\alpha(x+d))\exp\{-[x^2+\alpha^2(x+d)^2]/2\}}{x-\epsilon+\mathrm{i}\gamma}\,\mathrm{d}x\right|^2&\\ &=(2\pi)^2[(1-t^2)(1-s^2)]^{-1/2}\\ &\times\exp\left[-\epsilon^2\left(\frac{1-t}{1+t}+\frac{\alpha^2(1-s)}{1+s}\right)+\gamma^2\left(\frac{1+t}{1-t}+\frac{\alpha^2(1+s)}{1-s}+\frac{\alpha^2d(2\epsilon+d)(s-1)}{s+1}\right]\end{aligned}. \tag{43}$$

We recognize this generating function (with $c=\epsilon-\mathrm{i}\gamma$) as that for:

$$|H_n(c)H_m(\alpha(c+d))\exp\{-[c^2+\alpha^2(c+d)^2]/2\}|^2. \tag{44}$$

This generating function has been given since it has immediate application to the theory of vibrational excitation by Herzenberg and Mandl (1962); which though not quite so detailed as that of Birtwistle and Herzenberg (1971), has advantages in certain circumstances. In practice, to obtain the individual integrals, one would start with equation (42) and use recurrence.

7. Conclusions

It has been shown that generating functions exist for some classes of integrals involving Hermite functions and the problem of obtaining them in explicit form has been reduced to an algebraic one in some cases and to an application of the theory of two complex variables in others. Some previously unknown generating functions have been obtained.

References

Birtwistle D T and Herzenberg A 1971 *J. Phys. B: Atom. Molec. Phys.* **4** 53–70
Birtwistle D T and Modinos A 1972 *J. Phys. B: Atom. Molec. Phys.* **5** 445–65
Cuthill E H and Varga R S 1959 *J. Ass. Comput. Mach.* **6** 236–44
Dubé L and Herzenberg A 1975 *Phys. Rev.* A **11** 1314–25
Erdélyi (ed.) 1954 *Tables of Integral Transforms* vol. 2 (New York: McGraw-Hill)
Evans D J 1971 *Comput. J.* **14** 444–6
Evans D J and Atkinson L V 1970 *Comput. J.* **13** 323–4
Herzenberg A and Mandl F 1962 *Proc. R. Soc.* A **270** 48–71
Manneback C 1951 *Physica* **17** 1001–10
Mehler F G 1866 *J. Math., Lpz.* **66** 161–76
Mnatsakanyan A Kh 1971 *Opt. Spectrosc.* **30** 544–546 (1971 *Opt. Spektrosk.* **30** 1015–18)
Mnatsakanyan A Kh and Naidis G V 1975 *Sov. Phys.-Tech. Phys.* **19** 1113–15 (1974 *Zh. Tekh. Fiz.* **44** 1785–7)
Reuter G E H 1949 *J. Lond. Math. Soc.* **24** 159–60
Smith W L 1969 *J. Phys. B: Atom. Molec. Phys.* **2** 1–4, corrigendum 908
Sulzer P and Wieland K 1952 *Helv. Phys. Acta* **25** 653–66
Temperton C 1975 *J. Comput. Phys.* **19** 317–23
Turnbull H W and Aitken A C 1945 *Theory of Canonical Matrices* (London: Blackie)
Whittaker E T and Watson G N 1927 *A Course of Modern Analysis* (Cambridge: Cambridge University Press)