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Generating functions for integrals involving harmonic oscillator functions

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Abstract. Some generating functions involving harmonic oscillator functions are obtained as Lauricella functions and Appell functions.

1. Introduction

In my recent paper (Birtwistle 1977), to which I shall frequently refer and therefore refer to as B, I derived some new results on harmonic oscillator functions including the evaluation in closed form of generating functions of the type in equation (5) below. This work has been taken up by Labarthe (1978) who has introduced a graphical method with the aim of facilitating the manipulations. Dubé and Herzenberg (1975), Domcke and Cederbaum (1977) and Birtwistle and Modinos (1972) have applications of expressions of a similar type.

In B I also pointed out that progress could be made in obtaining generating functions for more general integrals involving Hermite functions which are of interest in mathematical physics and are of the class defined by equation (6) below. The requirement for more general results is illustrated in Birtwistle and Herzenberg (1971) and Holstein (1978). I suggested a result which could be used (Turnbull and Aitken 1945). Since then I have become aware of a powerful result obtained by Carlson (1972) which expresses the required quantities in terms of Lauricella (1893) functions. Section 2 is the statement of this theorem. In § 3 it is shown how Carlson's theorem can be used to obtain new generating functions. Some specific examples are worked out in detail in § 4.

2. Carlson's theorem

For $\mathbf{P}$ and $\mathbf{A}$ real symmetric $n \times n$ matrices and $\mathbf{A}$ being positive definite,

$$\int_{\{-\infty\}}^{\{\infty\}} (\boldsymbol{x}'\mathbf{P}\boldsymbol{x})^{\nu} \exp(-\boldsymbol{x}'\mathbf{A}\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}$$

$$= \pi^{n/2}\Gamma(\nu + n/2)R_{\nu}(\tfrac{1}{2}, \ldots, \tfrac{1}{2}; \lambda_1, \ldots, \lambda_n)/\Gamma(n/2)|\mathbf{A}|^{1/2} \qquad (1)$$

where the λ_i are the eigenvalues of $\mathbf{PA}^{-1}$ and one of the following conditions is satisfied:

(i) **P** is positive definite and $\mathrm{Re}(\nu) > -n/2$
or that,

(ii) **P** is non-negative define and $\mathrm{Re}(\nu) > 0$
or that,

(iii) **P** is real and symmetric and ν is a non-negative integer.

Here,

$$
\begin{aligned}
R_\nu(b_1, \ldots, b_n; z_1, \ldots, z_n) \\
&= F_D^{(n)}(\nu, b_1, \ldots, b_n; b_1 + \ldots b_n; 1 - z_1, \ldots, 1 - z_n) \\
&= \sum \frac{(\nu, m_1 + \ldots + m_n)(b_1, n_1) \ldots (b_n, m_n)}{(b_1 + \ldots + b_n, m_1 + \ldots + m_n)} \\
&\times \frac{(1 - z_1)^{m_1} \times \ldots \times (1 - z_n)^{m_n}}{m_1! \ldots m_n!}.
\end{aligned} \tag{2}
$$

$R_\nu(.)$ is the symmetrised form of Lauricella's function (Lauricella 1893) which was introduced by Carlson (1963) and is symmetric under permutation of the subscripts $1 \ldots n$ and is a homogeneous function of degree $-\nu$ in $z_1, \ldots, z_n$.

$$
\begin{aligned}
(\lambda, k) &= (\lambda)_k \\
&= \Gamma(\lambda + k)/\Gamma(\lambda) \qquad k \geqslant 0 \\
&= (-1)^k/(1 - \lambda, k) \qquad k < 0.
\end{aligned} \tag{3}
$$

In the case of two variables the Lauricella functions reduce to Appell functions (Appell and Kampé de Fériet, 1926) and in particular

$$
F_D^{(2)}(\alpha, \beta, \beta'; \gamma; x, y) = F_1(\alpha; \beta, \beta'; \gamma; x, y) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(\alpha)_{m+n}(\beta)_m(\beta')_n x^m y^n}{m! n! (\gamma)_{m+n}}. \tag{4}
$$

Carlson's theorem is an extension of the one which I used before. In the next section some possible applications are considered.

3. The applications of Carlson's theorem

As far as possible the notation is the same as in B. The ket$|n\rangle$ is understood to be $|n\rangle \equiv |n, \alpha, d\rangle$, the states being normalised harmonic oscillator states with scaling parameter α and centred at $-d$. The generating functions previously evaluated were of the form,

$$
S_m = \sum_{n=0}^{\infty} \sum_{\text{all } \lambda_i = 0}^{\infty} \left\langle n \middle| \prod_{i=2}^{m} |\lambda_i\rangle t_i^{\lambda_i} \langle \lambda_i | t_1^n \middle| n \right\rangle, \tag{5}
$$

and those of this paper are of the form

$$
T_m = \sum_{n=0}^{\infty} \sum_{\text{all } \lambda_i = 0}^{\infty} \langle n | Q_n \prod_{i=2}^{m} (|\lambda_i\rangle t_i^{\lambda_i} \langle \lambda_i | Q_i) t_1^n | n \rangle. \tag{6}
$$

Here, as is usual in quantum theory,

$$\langle n|Q|\mu\rangle = \int_{-\infty}^{\infty} \psi_n(\alpha_n(x+\mathrm{d}_n))Q(x)\psi_\mu(\alpha_\mu(x+\mathrm{d}_\mu))\,\mathrm{d}x, \tag{7}$$

with the ψ_n being normalised harmonic oscillator functions. The elements of the matrix $\mathbf{A}$ are to be defined as in B and originate with the Mehler formula (Mehler 1866). In order to use Carlson's (1972) theorem we have to eliminate the term in the argument of the Gaussian which is linear in $\boldsymbol{x}$. Since $\mathbf{A}$ is symmetric, this can be done by transforming to

$$\boldsymbol{q} = \boldsymbol{x} - \tfrac{1}{2}\mathbf{A}^{-1}\boldsymbol{b}, \tag{8}$$

and changing the constant term in the Gaussian from the c of B to c',

$$c' = c + \tfrac{1}{4}\boldsymbol{b}'\mathbf{A}^{-1}\boldsymbol{b}. \tag{9}$$

The expression equation (9) is the argument of the Gaussian in the final result as calculated in B and evaluated in some individual cases by previous authors (Manneback 1951, Mnatsakanyan 1971, Mnatsakanyan and Naidis 1975). Hence the generating functions contain the common Gaussian factor as it is intuitively obvious that they must. We have freedom to choose matrix $\mathbf{P}$ and index ν, subject to the conditions of equation (1), to derive a variety of results.

4. Some specific examples

Consider the instance when two sets of states are involved. Let Greek letters be understood to be associated with one set of Hermite functions, and Latin letters with a second set, displaced from the first and with a different frequency (scaling). Define

$$\lambda = (M_n\omega_n/M_\mu\omega_\mu)^{1/2} = \alpha_n/\alpha_\mu$$

where M_μ is the reduced mass and ω_n the angular frequency of the state n and M_μ and ω_μ are those for the state μ. Results are much easier to obtain in the case when $\lambda = 1$, which corresponds to the states having the same vibration frequency, but then they are of very restricted value in molecular physics. However, without loss of generality we may set $\alpha_\mu = 1$ so that $\lambda = \alpha_n = \alpha$ in the following.

The generating function

$$\begin{aligned} S_2(s,t) &= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} S^n t^\mu |\langle n|\mu\rangle|^2 \\ &= 2\lambda[(1-s^2)(1-t^2)(1+\lambda^2)^2 + 4\lambda^2(s-t)^2]^{-1/2} \\ &\quad\times \exp\left(\frac{-2\Lambda(1-s)(1-t)}{(1+s)(1-t)+\lambda^2(1-s)(1+t)}\right) \end{aligned} \tag{10}$$

was obtained and used for $\lambda = 1$ by Manneback (1951) and in the form above for general λ by Mnatsakanyan (1971). Here $\Lambda = \frac{1}{2}\lambda^2(\mathrm{d}_n - \mathrm{d}_\mu)^2$. Now combining the results of my previous paper (Birtwistle 1977) with Carlson (1972) we can obtain the analogous generating functions:

$$T_2(s,t) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} s^n t^\mu |\langle n|q|\mu\rangle|^2. \tag{11}$$

The matrix **A** is defined by

$$\begin{aligned} a_{11} = a_{22} &= \tfrac{1}{2}\left(\frac{\alpha^2(1+s^2)}{(1-s^2)} + \frac{(1+t^2)}{(1-t^2)}\right) \\ a_{12} = a_{21} &= -\left(\frac{\alpha^2 s}{1-s^2} + \frac{t}{1-t^2}\right) \end{aligned} \tag{12}$$

and

$$b_1 = b_2 = -\alpha^2\, \mathrm{d}_n \frac{(1-s)}{(1+s)} - \mathrm{d}_\mu \frac{(1-t)}{(1+t)}.$$

Note that in condensing my earlier work for publication I incorrectly introduced a minus sign into the definition of all of the elements of **A**. The general definition in B holds only for $n > 2$. Take

$$\mathbf{P}_1 = \begin{pmatrix} 0 & \tfrac{1}{2} \\ \tfrac{1}{2} & 0 \end{pmatrix}. \tag{13}$$

The eigenvalues of $\mathbf{P}_1\mathbf{A}^{-1}$ are found to be,

$$\lambda_1(s, t) = \frac{-(1+s)(1+t)}{[(1+s)(1-t) + \alpha^2(1-s)(1+t)]} \tag{14}$$

and

$$\lambda_2(s, t) = -\lambda_1(-s, -t) = -(4\lambda_1(s, t)|\mathbf{A}|)^{-1}$$

to give

$$\begin{aligned} \sum_{n=0}^{\infty} \sum_{\mu=0}^{\infty} s^n t^\mu |\langle n|q^\nu|\mu\rangle|^2 \\ &= S_2(s, t)\Gamma(\nu+1)R_\nu(\tfrac{1}{2}, \tfrac{1}{2}; \lambda_1, \lambda_2) \\ &= S_2(s, t)\Gamma(\nu+1)F_1(\nu, \tfrac{1}{2}, \tfrac{1}{2}; 1; 1-\lambda_1, 1-\lambda_2). \end{aligned} \tag{15}$$

with λ_1, λ_2 given by equation (14), q by equation (8) and $S_2(s, t)$ by equation (10).

Now take

$$\mathbf{P}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{16}$$

so that

$$\mathbf{P}_2\mathbf{A}^{-1} = \mathbf{A}^{-1}. \tag{17}$$

Calculating the eigenvalues λ_3 and λ_4 we find

$$\begin{aligned} \lambda_3(s, t) &= -2\lambda_1(s, t) \\ \lambda_4(s, t) &= \lambda_3(-s, -t) \\ &= (\lambda_3(s, t)|\mathbf{A}|)^{-1} \end{aligned} \tag{18}$$

and hence the result

$$\sum_{n=0}^{\infty} \sum_{\mu=0}^{\infty} s^n t^\mu \langle n|q^2|\mu\rangle\langle\mu|n\rangle = \tfrac{1}{2}S_2(s, t)R_1(\tfrac{1}{2}, \tfrac{1}{2}, \lambda_3, \lambda_4). \tag{19}$$

In the case of equal frequencies the eigenvalues are given by equations (14) and (18) with λ_1 reducing to:

$$\lambda_1(s, t) = \frac{-(1+s)(1+t)}{2(1-st)}. \tag{20}$$

The apparent simplicity of these generating functions is to a certain extent deceptive because we have used the transformation equation (8) and therefore the operators have the unusual feature that they contain the auxiliary variables s and t. In the case just discussed in terms of the x of equation (7)

$$q = x - \frac{[\mathrm{d}_n\alpha^2(1-s)(1+t) + \mathrm{d}_\mu(1+s)(1-t)]}{[(1+s)(1-t) + \alpha^2(1-s)(1+t)]}. \tag{21}$$

This complication can be overcome by constructing the desired linear combination of generating functions. It should also be possible to derive recurrence schemes of the type obtained by Smith (1969).

5. Conclusions

It has been shown that some useful generating functions can be obtained in closed form in terms of Lauricella (1893) functions as symmetrised by Carlson (1963). There is a large body of results known for Lauricella functions, which for two variables are Appell functions and generating functions are known for them. This indicates that other useful results can be obtained, especially if the special methods for sparse matrices (Labarthe 1978) are used.

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References

Appell P and Kampé de Fériet J 1926 *Fonctions Hypérgéometriques: Polynomes d'Hermite* (Paris: Gauthier-Villars)
Birtwistle D T and Herzenberg A 1971 *J. Phys. B: Atom. Molec. Phys.* **4** 43–70
Birtwistle D T and Modinos A 1972 *J. Phys. B: Atom. Molec. Phys.* **5** 445–6
Birtwistle D T 1977 *J. Phys. A: Math. Gen.* **10** 677–87
Carlson B C 1963 *J. Math. Anal. Appl.* **7** 452–70
—— 1972 *C.R. Acad. Sci. Paris* **274** 1458–61
Domcke W and Cederbaum L S 1977 *Phys. Rev.* A **16** 1465–82
Dubé L and Herzenberg A 1975 *Phys. Rev.* A **11** 1314–25
Holstein T 1978 *Phil. Mag.* B **37** 49–62
Labarthe J-J 1978 *J. Phys. A: Math. Gen.* **11** 1009–15
Lauricella G 1893 *Rend. Circ. Mat. Palermo* **7** 111–58
Manneback C 1951 *Physica* **17** 1001–10
Mehler F G 1866 *J. Math. Lpz.* **66** 161–76
Mnatsakanyan A Kh 1971 *Opt. Spectrosc.* **30** 544–6
Mnatsakanyan A Kh and Naidis G V 1975 *Sov. Phys.-Tech. Phys.* **19** 1113–5
Smith W L 1969 *J. Phys. B: Atom. Molec. Phys.* **2** 1–4 (Corrigendum 908)
Turnbull H W and Aitken A C 1945 *Theory of Canonical Matrices* (London: Blackie) p 183