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LETTER TO THE EDITOR

Partial differential matrix equations for generalized hypergeometric functions

L E Wright, D S Onley and C W Soto Vargas
Physics Department, Ohio University, Athens, Ohio, 45701, USA

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Abstract. A method of handling a number of generalized hypergeometric functions in terms of first-order partial differential matrix equations is introduced. This method has many advantages in formal manipulations and in numerical integration. In particular, it allows investigation of the energy dependence of matrix elements arising in scattering problems in quantum mechanics.

Many functions, very common in the solution of wave equations of various kinds, are special cases of the Whittaker functions (Whittaker and Watson 1927) or its close relative the confluent hypergeometric function: a few examples are Bessel functions, Coulomb wavefunctions, Laguerre functions, and Airy functions. Also common in such problems are functions defined by integrals over products of Whittaker functions, some of which may be identified, for example Appell functions or Lauricella functions, but many are nameless and have few recorded properties. We show here methods of handling such functions in terms of first-order differential matrix equations which have many advantages both in formal and numerical analysis and which are also capable of encompassing a much larger family of functions than simply those mentioned above.

The Whittaker functions are normally defined as solutions of the differential equation

$$\frac{d^2w}{dz^2}+\left(\frac{(\frac{1}{4}-\mu^2)}{z^2}+\frac{\kappa}{z}-\frac{1}{4}\right)w=0. \tag{1}$$

The notation $M_{\kappa,\mu}$ denotes the solution with the property

$$M_{\kappa,\mu}(z)\approx z^{\mu+\frac{1}{2}}, \qquad \text{for } z\approx 0 \tag{2}$$

so that of the two solutions of (1), $M_{\kappa,\mu}$ and $M_{\kappa,-\mu}$, one is regular at the origin.

Whittaker functions also arise in the general solution of the equation

$$\frac{dU}{dx}=\left(\frac{1}{x}A-B\right)U \tag{3}$$

where A, B, U are 2×2 matrices. One of the simplest forms involving these functions is when

$$A=\begin{pmatrix} -(\kappa+\frac{1}{2}) & \mu+\kappa+\frac{1}{2} \\ \mu-\kappa-\frac{1}{2} & \kappa+\frac{1}{2} \end{pmatrix}, \qquad B=\begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \tag{4}$$

in which case a solution is

$$U_{\kappa,\mu}(x)=x^{-\frac{1}{2}}\begin{pmatrix} M_{\kappa,\mu}(x) & \dfrac{\kappa+\mu+\frac{1}{2}}{\kappa-\mu+\frac{1}{2}}M_{\kappa,-\mu}(x) \\ M_{\kappa+1,\mu}(x) & M_{\kappa+1,-\mu}(x) \end{pmatrix}.$$

This solution also arises in the separation in polar coordinates of the Dirac equation for an electron in a Coulomb field (Rose 1961).

Also of interest are functions defined by integrals over products of n Whittaker functions:

$$\mathscr{F}(\{\kappa_i\},\{\mu_i\},\{k_i\})=\int_{(0)}^{\infty} M_{\kappa_1\mu_1}(k_1x)M_{\kappa_2\mu_2}(k_2x)\dots M_{\kappa_n\mu_n}(k_nx)\,\mathrm{d}x \tag{5}$$

where the notation (0) indicates the subtraction of the contribution of poles which may occur at the origin. For $n=1, 2$, and 3 the functions of (5) are identifiable as examples of the Gauss hypergeometric function, Appell functions and Lauricella functions (Appell and Fériet 1926), the last two of which are functions of some complexity defined by n coupled partial differential equations of second order in n variables. We define a matrix function corresponding to that defined in (5):

$$\Gamma(\{\kappa_i\},\{\mu_i\},\{k_i\})=\int_{(0)}^{\infty} U_{\kappa_n\mu_n}(k_nx)\otimes\dots\otimes U_{\kappa_2\mu_2}(k_2x)\otimes U_{\kappa_1\mu_1}(k_1x)\,\mathrm{d}x$$

which is evidently a matrix, of order $2^n\times 2^n$, whose elements are all functions of the type defined in (5). We show next that this matrix function satisfies equations of the form

$$\frac{\partial\Gamma}{\partial k_i}=T_i\Gamma \qquad i=1,2,\dots,n. \tag{6}$$

First notice that the outer product

$$W=U_{\kappa_n\mu_n}(k_nx)\otimes\dots\otimes U_{\kappa_2\mu_2}(k_2x)\otimes U_{\kappa_1\mu_1}(k_1x) \tag{7}$$

wherein each function U is a solution of an equation of the type (3), is itself a solution of an equation of the same form but with A and B matrices of order 2^n (here denoted by $\mathscr{A}$, $\mathscr{B}$) and defined by

$$\mathscr{A}=A_n\otimes I_{2n-2}+I_2\otimes A_{n-1}\otimes I_{2n-4}+\dots+I_{2n-2}\otimes A_1$$

$$\mathscr{B}=k_nB\otimes I_{2n-2}+k_{n-1}I_2\otimes B\otimes I_{2n-4}+\dots+k_1I_{2n-2}\otimes B.$$

Here I_m denotes the $m\times m$ unit matrix. Each matrix A (see (4)) is a function of κ, μ and we have abbreviated $A(\kappa_i,\mu_i)$ by A_i simply. Consequently $\mathscr{A}$ is a function of $\{\kappa_i\}$ and $\{\mu_i\}$ only, whereas $\mathscr{B}$ is a function of $\{k_i\}$ only. Now adopting the notation of Onley (1972) and Sud *et al* (1976) we write W defined in (7) as a function of these two matrices and the scalar x

$$W=W(\mathscr{A},\mathscr{B},x)$$

and, from the same references, we will denote the integral by

$$\Gamma(\mathscr{A}+1,\mathscr{B})=\int_{(0)}^{\infty} W(\mathscr{A},\mathscr{B},x)\,\mathrm{d}x. \tag{8}$$

Evidently, from (3)

$$\frac{\partial W}{\partial k_i} = U_n(k_n x) \otimes \ldots \otimes (A_i/k_i - Bx) U_i(k_i x) \otimes \ldots \otimes U_1(k_1 x)$$

and using the following properties taken from Onley (1972):

$$xW(\mathscr{A}, \mathscr{B}, x) = W(\mathscr{A}+1, \mathscr{B}, x) \qquad \mathscr{B}^{-1}\mathscr{A}\Gamma(\mathscr{A}, \mathscr{B}) = \Gamma(\mathscr{A}+1, \mathscr{B}),$$

it is straightforward to see that

$$\frac{\partial \Gamma}{\partial k_i} = \left(\frac{1}{k_i} I_{2n-2i} \otimes A_i \otimes I_{2i-2} - I_{2n-2i} \otimes B \otimes I_{2i-2} \mathscr{B}^{-1}(\mathscr{A}+1)\right)\Gamma. \tag{9}$$

In (9), aside from the explicit appearance of k_i, the only function of the $\{k_i\}$ is $\mathscr{B}$ which is homogeneous and linear in these variables. The equation is evidently homogeneous in $\{k_i\}$.

To show the connection between the elements of Γ and the higher-order hypergeometric series, we consider the case $n = 2$. Writing the Whittaker functions in terms of the confluent hypergeometric series, (5) becomes

$$\begin{aligned} &\mathscr{F}(\kappa_1, \kappa_2, \mu_1, \mu_2, k_1, k_2) \\ &\quad = \int_{(0)}^{\infty} \exp[-\tfrac{1}{2}(k_1+k_2)x] k_1^{\mu_1+\frac{1}{2}} k_2^{\mu_2+\frac{1}{2}} x^{\mu_1+\mu_2+1} \\ &\qquad \times {}_1F_1(\tfrac{1}{2}+\mu_1-\kappa_1, 1+2\mu_1, k_1 x)\, {}_1F_1(\tfrac{1}{2}+\mu_2-\kappa, 1+2\mu_2, k_2 x)\, \mathrm{d}x \end{aligned}$$

which is integrable term by term (provided $\mathrm{Re}(k_1+k_2) > 0$) yielding

$$\begin{aligned} &\mathscr{F}(\kappa_1, \kappa_2, \mu_1, \mu_2, k_1, k_2) \\ &\quad = \frac{2}{k_1+k_2} \Gamma(\mu_1+\mu_2+1) x_1^{\mu_1+\frac{1}{2}} x_2^{\mu_2+\frac{1}{2}} \\ &\qquad \times F_2(\mu_1+\mu_2+1, \tfrac{1}{2}+\mu_1-\kappa_1, \tfrac{1}{2}+\mu_2-\kappa_2, 1+2\mu_1, 1+2\mu_2; x_1, x_2). \end{aligned} \tag{10}$$

In (10) $x_i = 2k_i/(k_1+k_2)$ and F_2 is one of the double hypergeometric functions of Appell:

$$F_2(\alpha, a_1, a_2, b_1, b_2; x_1, x_2) = \sum_{m,n} \frac{(\alpha)_{m+n}(a_1)_m(a_2)_n}{(b_1)_m(b_2)_n m!\,n!} x_1^m x_2^n.$$

Equation (6) has the regular solution

$$\Gamma = \begin{pmatrix} \mathscr{F}(\kappa_1, \kappa_2, \mu_1, \mu_2; x_1, x_2) \\ \mathscr{F}(\kappa_1+1, \kappa_2, \ldots) \\ \mathscr{F}(\kappa_1, \kappa_2+1, \ldots) \\ \mathscr{F}(\kappa_1+1, \kappa_2+1, \ldots) \end{pmatrix}$$

(where $\mathscr{F}(\ldots)$ is defined in (5) and the arguments omitted are the same in all rows). This equation is evidently a convenient alternative to define $\mathscr{F}(\ldots)$ and its companion functions. It is interesting to see how this is related to the partial differential equations satisfied by the Appell function:

$$x_1(1-x_1)\frac{\partial^2 F_2}{\partial x_1^2}-x_1x_2\frac{\partial^2 F_2}{\partial x_1\partial x_2}+[b_1-(\alpha+a_1+1)x_1]\frac{\partial F_2}{\partial x_1}-a_1x_2\frac{\partial F_2}{\partial x_2}-\alpha a_1F_2=0$$

$$x_2(1-x_2)\frac{\partial^2 F_2}{\partial x_2^2}-x_1x_2\frac{\partial^2 F_2}{\partial x_1\partial x_2}+[b_2-(\alpha+a_2+1)x_2]\frac{\partial F_2}{\partial x_2}-a_2x_1\frac{\partial F_2}{\partial x_1}-\alpha a_2F_2=0.$$

These equations may be rendered into the form of coupled first-order partial differential equations in four functions—for example F_2, $\partial F_2/\partial x_1$, $\partial F_2/\partial x_2$, and $\partial^2 F_2/\partial x_1\partial x_2$, although the resulting equations are not particularly concise. Simpler forms for such equations arise from the techniques used here. To show this for the present case we begin by identifying the equation satisfied by the confluent function ${}_1F_1(a, b, x)$ and its contiguous neighbour ${}_1F_1(a+1, b, x)$. Replacing the matrices A and B in (4) with the matrices

$$C=\begin{pmatrix}-a & a\\ b-a-1 & -(b-a-1)\end{pmatrix},\qquad D=\begin{pmatrix}0 & 0\\ 0 & -1\end{pmatrix}$$

we find the regular solution

$$V(a,b,x)=\begin{pmatrix}{}_1F_1(a,b,x)\\ {}_1F_1(a+1,b,x)\end{pmatrix}.$$

Now,

$$\Gamma(\mathscr{C}+1,\mathscr{D})=\int_{(0)}^{\infty}\mathrm{e}^{-u}u^{\alpha}V(a_2,b_2,x_2u)\otimes V(a_1,b_1,x_1u)\,\mathrm{d}u$$

where

$$\mathscr{C}=I_2\otimes C_1+C_2\otimes I_2+\alpha I_4$$

$$\mathscr{D}=x_1I_2\otimes D+x_2D\otimes I_2+I_4$$

has the elements (regular column only)

$$\Gamma=\begin{pmatrix}F_2(\alpha,a_1,a_2,b_1,b_2;x_1,x_2)\\ F_2(\alpha,a_1+1,a_2,\ldots)\\ F_2(\alpha,a_1,a_2+1,\ldots)\\ F_2(\alpha,a_1+1,a_2+1,\ldots)\end{pmatrix}.$$

This matrix function satisfies (6) with

$$T_1=\frac{I_2\otimes C_1}{x_1}-(I_2\otimes D)\mathscr{D}^{-1}(\mathscr{C}+I)$$

$$T_2=\frac{C_2\otimes I_2}{x_2}-(D\otimes I_2)\mathscr{D}^{-1}(\mathscr{C}+I).$$

As an example of how these considerations may be applied, we consider an $n=3$ case corresponding to the product of incident and final wavefunctions and a Green function that might arise in scattering problems in quantum mechanics. Typically the incident energy (momentum) $E_1(P_1)$ is fixed and one requires matrix elements as a function of energy loss, ω, or momentum transfer, k, of the projectile where energy conservation requires $\omega = E_1 - E_2$, $E_2(P_2)$ being the final projectile energy (momentum). In such cases, the Γ matrix of (8) is an 8×8 array of Lauricella functions, and satisfies

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}\omega} = \frac{\partial\Gamma}{\partial k}\frac{\partial k}{\partial\omega} + \frac{\partial\Gamma}{\partial P_2}\frac{\partial P_2}{\partial\omega} \tag{11}$$

where the partial differentials of Γ are given by equations of the type (9). Equation (11) is straightforwardly solved by numerical integration given the initial values of Γ, thereby allowing the evaluation of the matrix elements over a complete energy range, including regions where direct evaluation of Γ may not be feasible.

To summarize, we have introduced first-order partial differential matrix equations whose solutions correspond to various generalized hypergeometric functions in n variables. The matrix representation of these functions is particularly convenient in formal manipulations and in the application of numerical integration techniques. Furthermore, we suggest that all generalized hypergeometric functions may be usefully treated as solutions of equations of the type (6).

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