Symmetry and Separation of Variables

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Volume 4

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Symmetry and Separation of Variables

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Editor's Statement

A large body of mathematics consists of facts that can be presented and described much like any other natural phenomenon. These facts, at times explicitly brought out as theorems, at other times concealed within a proof, make up most of the applications of mathematics, and are the most likely to survive changes of style and of interest.

This ENCYCLOPEDIA will attempt to present the factual body of all mathematics. Clarity of exposition, accessibility to the non-specialist, and a thorough bibliography are required of each author. Volumes will appear in no particular order, but will be organized into sections, each one comprising a recognizable branch of present-day mathematics. Numbers of volumes and sections will be reconsidered as times and needs change.

It is hoped that this enterprise will make mathematics more widely used where it is needed, and more accessible in fields in which it can be applied but where it has not yet penetrated because of insufficient information.

Anyone who has ever had to solve a differential equation is familiar with separation of variables. Mostly, this method is remembered as a bag of tricks at the borderline of mathematics.

Professor Miller has given the first systematic treatment of this method. He shows how separation of variables relates to one of the central fields of today's mathematics and mathematical physics; namely, the theory of Lie algebras.

This volume is the first in the Section dealing with the theory of those special functions which occur in the practice of mathematics.

GIAN-CARLO ROTA

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Foreword

This is the first in a series of books that will try to show how and why special functions arise in many applications of mathematics. The elementary transcendental functions, such as the exponential, its inverse, the logarithm, and the trigonometric functions, form part of the working tools of all mathematicians and most users of mathematics. There was a time when knowledge of some of the higher transcendental functions was almost as widespread. For example, there were a surprisingly large number of books written on elliptic functions in the last half of the nineteenth century, and esoteric facts about Bessel functions and Legendre functions were regularly set as tripos problems. However, knowledge of these functions and the few other very useful special functions is no longer as widespread, and it has even been possible for important special functions to arise in applications and be studied for twenty-five years or more without any of the people studying them being aware that some of the results they rediscovered were found about a hundred years earlier. This has occurred in the last forty years with what are called $3-j$ symbols. These functions occur when studying the decomposition of the direct product of two irreducible representations of $SU(2)$. Since a knowledge of hypergeometric series was not as widespread as it should be, it has only recently been realized that one of the orthogonality relations for $3-j$ symbols is the same as the orthogonality for a set of polynomials that was found by Tchebychef in 1875 and that Tchebychef had some useful formulas for these polynomials that still have not been published in the physics literature, where most of the development of $3-j$ symbols has occurred. Similarly, a symmetry relation for the $3-j$ symbols that was found by Regge in 1958 had been given by Whipple in 1923 and even earlier by Thomae in 1879. The first of the symmetries for these functions was stated by Kummer in 1836. If these results were easy to derive and

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could be found by anyone who needs them, then there would be no reason to worry about old results getting lost. However, this is often not the case, and was definitely not true with respect to Regge's symmetry. The $3-j$ symbols had been studied by many people in the period from 1930 to 1958, and every one of them had missed this symmetry.

The lack of information transfer between mathematicians and users of mathematics goes both ways; this can also be illustrated by a similar example. In 1942 Racah published an important orthogonality relation for functions that are now called $6-j$ symbols or Racah coefficients. He also found an important representation for these functions as a single sum. They arise naturally as a fourfold sum. When Racah's single-sum expression is used in his orthogonality relation, and a transformation formula of Whipple is used on the $6-j$ symbol (Racah had rediscovered this transformation), a new set of orthogonal polynomials arises which had been completely missed in the mathematics literature. In fact the situation was worse than that; not only had this set of orthogonal polynomials not been discovered, there were a number of theorems that seemed to say that the existing set of orthogonal polynomials in one variable were all the orthogonal polynomials in one variable that would have useful explicit formulas. This was not true, as the polynomials buried in Racah's work show.

The most important lesson to be learned from this example is that people with different backgrounds need to talk to each other, since mathematics does not come in isolated parts that are unrelated. This series of books is one attempt to try to show how one part of mathematics relates to other parts, and how it can be used to solve problems of interest to scientists with many different backgrounds. The rest of the Foreword will be a short outline of our current view of special functions. Since there are a number of important special functions, this summary will be given in approximately the order in which the functions were discovered. One fact which will surprise many people is that our current view of some subjects has changed only slightly since the first deep results. We write in a more modern language, but most of the ideas we use were present at a very early time.

When applications are considered, the most important special functions are the hypergeometric functions. A generalized hypergeometric series is a series

$$\sum_{n=0}^{\infty} a_n$$

with a_{n+1}/a_n a rational function of n. This rational function is usually factored as

$$\frac{a_{n+1}}{a_n}=\frac{(n+a_1)(n+a_2)\cdots(n+a_p)}{(n+b_1)(n+b_2)\cdots(n+b_q)}\frac{x}{(n+1)},$$

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so that

$$a_n = \frac{(a_1)_n \cdots (a_p)_n}{(b_1)_n \cdots (b_q)_n} \frac{x^n}{n!}.$$

The shifted factorial $(a)_n$ is defined by

$$\begin{aligned}&(a)_n = a(a+1)\cdots(a+n-1), \qquad n=1,2,\ldots,\\&(a)_0 = 1.\end{aligned}$$

The series $\sum_{n=0}^{\infty} a_n$ is written as

$${}_pF_q\left(\begin{matrix} a_1,\ldots,a_p \\ b_1,\ldots,b_q \end{matrix}; x\right) = \sum_{n=0}^{\infty} \frac{(a_1)_n \ldots (a_p)_n}{(b_1)_n \ldots (b_q)_n} \frac{x^n}{n!}.$$

This series converges for all complex x when $p \leqslant q$ and $|x|<1$ when $p=q+1$. Among the special cases are

$$\exp(x) = {}_0F_0(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!};$$

$$(1-x)^{-a} = {}_1F_0\left(\begin{matrix} a \\ \text{—} \end{matrix}; x\right) = \sum_{n=0}^{\infty} \frac{(a)_n}{n!} x^n \qquad (|x|<1);$$

$$\sin x = x_0F_1\left(\begin{matrix} \text{—} \\ \frac{3}{2} \end{matrix}; \frac{-x^2}{4}\right);$$

$$\cos x = {}_0F_1\left(\begin{matrix} \text{—} \\ \frac{1}{2} \end{matrix}; \frac{-x^2}{4}\right);$$

$$\log(1+x) = x_2F_1\left(\begin{matrix} 1,1 \\ 2 \end{matrix}; -x\right) \qquad (|x|<1);$$

$$\arctan x = x_2F_1\left[\begin{matrix} \frac{1}{2},1 \\ \frac{3}{2} \end{matrix}; -x^2\right] \qquad (|x|<1);$$

$$\arcsin x = x_2F_1\left[\begin{matrix} \frac{1}{2},\frac{1}{2} \\ \frac{3}{2} \end{matrix}; x^2\right] \qquad (|x|<1);$$

$$\cos \pi x = {}_2F_1\left(\begin{matrix} x,-x \\ \frac{1}{2} \end{matrix}; 1\right).$$

The last example is particularly important, for it suggests that the parameters that occur in hypergeometric series can play a more important role in

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the study of hypergeometric series than that of just enabling us to distinguish between different series. Gauss was probably the first person to realize this; we will return to his results after describing some earlier work of Wallis and Euler that is necessary before we can see why this last formula holds.

The factorial function $n! = 1 \cdot 2 \cdot \cdots \cdot n$ occurs as soon as one considers the binomial theorem. The easiest extension of $n!$ is the shifted factorial $(a)_n$ defined earlier. Clearly, $n! = (1)_n$. However, it does not solve an interesting question, what is $(\frac{1}{2})!$? This question was solved by Euler when he introduced $\Gamma(x)$. His original expression was an infinite product, but he also gave an integral representation which is equivalent to

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t}\, dt.$$

This integral is our usual starting point when developing properties of $\Gamma(x)$, but there is something to be said for Euler's product or other definitions which define the gamma function directly for all x and not just for $\operatorname{Re} x > 0$, as in the integral. One such definition is

$$\frac{1}{\Gamma(x)} = x e^{\gamma x} \prod_{n=1}^{\infty} \left(1 + \frac{x}{n}\right) e^{-x/n}$$

where

$$\gamma = \lim_{n\to\infty} \left(1 + \frac{1}{2} + \cdots + \frac{1}{n} - \log n\right).$$

Another, which was found by Euler but is usually attributed to Gauss, is

$$\frac{1}{\Gamma(x)} = \lim_{n\to\infty} \frac{(x)_n}{(1)_n} n^{1-x}.$$

Euler used the gamma function to evaluate the beta function integral

$$B(x,y) = \int_0^1 t^{x-1} (1-t)^{y-1}\, dt$$

as

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}.$$

It is very easy to see that this implies $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. In fact, Euler's original

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definition of the gamma function reduces (after using some simple algebra) to Wallis's infinite product for π when $x=\frac{1}{2}$.

In the nineteenth century many different integral representations were given for $\Gamma(x)$, and Hankel proved that it did not satisfy a differential equation with algebraic coefficients. It does satisfy the difference equation $\Gamma(x+1)=x\Gamma(x)$, but this is not a sufficiently strong condition to determine $\Gamma(x)$. A natural condition that forces the solution to be unique was found by Bohr and Mollerup: $\log\Gamma(x)$ is convex for $x>0$. The current generation of mathematicians is quite interested in structural conditions, and this theorem is a beautiful example of the type of result that is held in high regard by contemporary mathematicians. It is a very pretty theorem, and it is useful; but we must not forget that the real reason the gamma function is studied is because it is so useful. It occurs so often that we are forced to consider it. This is just one of many examples of the way mathematical aesthetics and utility force us in the same path. Why this happens is still a mystery.

Study of the factorial and the gamma function has led to the development of a number of general mathematical ideas that have been useful elsewhere. One of the most fruitful is the notion of an asymptotic expansion. Stirling found a method of computing $n!$ for large n. The series he obtained does not converge, but it can still be used to obtain very accurate values of $n!$. Euler's formula

$$\Gamma(x)\Gamma(1-x)=\frac{\pi}{\sin \pi x}$$

can be used to give an analytic continuation of the gamma function from $\mathrm{Re}\, x>0$ to $\mathrm{Re}\, x<1$, $x\neq 0, -1,\ldots$. When used with one of the infinite products for $\Gamma(x)$ it gives Euler's product

$$\frac{\sin \pi x}{\pi x}=\prod_{n=1}^{\infty}\left(1-\frac{x^2}{n^2}\right).$$

This product, the one given earlier for $1/\Gamma(x)$, and some further products for elliptic functions and theta functions which will be mentioned later led Weierstrass to his theorem on canonical products for entire functions, and the logarithmic derivatives of the product formulas led Mittag-Leffler to his expansion theorem for meromorphic functions.

To return to hypergeometric series, Gauss evaluated

$$\sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{(c)_n n!}={}_2F_1\left(\begin{matrix}a,b\\c\end{matrix};1\right)=\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)},\qquad \mathrm{Re}(c-a-b)>0.$$

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When $c=\frac{1}{2}$, $a=x$, $b=-x$, this is

$$ {}_2F_1\left(\begin{matrix} x,-x \\ \frac{1}{2} \end{matrix};1\right)=\frac{\left[\Gamma\left(\frac{1}{2}\right)\right]^2}{\Gamma\left(\frac{1}{2}-x\right)\Gamma\left(\frac{1}{2}+x\right)}=\sin\pi\left(\tfrac{1}{2}+x\right)=\cos\pi x. $$

Euler was the first to study ${}_2F_1\left(\begin{matrix} a,b \\ c \end{matrix};x\right)$ in the general case. He found a second-order differential equation it satisfies, and gave the transformation formula

$$ {}_2F_1\left(\begin{matrix} a,b \\ c \end{matrix};x\right)=(1-x)^{c-a-b}\,{}_2F_1\left(\begin{matrix} c-a,c-b \\ c \end{matrix};x\right) $$

and the integral representation

$$ {}_2F_1\left(\begin{matrix} a,b \\ c \end{matrix};x\right)=\frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1(1-xt)^{-a}t^{b-1}(1-t)^{c-b-1}\,dt. $$

Pfaff, in the course of editing some of Euler's posthumous papers, found two more transformation formulas. He stated both only in the case in which the series terminates, but one extends immediately to the non-terminating case. They are

$$ {}_2F_1\left(\begin{matrix} a,b \\ c \end{matrix};x\right)=(1-x)^{-a}\,{}_2F_1\left(\begin{matrix} a,c-b \\ c \end{matrix};\frac{x}{x-1}\right) $$

and

$$ {}_2F_1\left(\begin{matrix} -n,b \\ c \end{matrix};x\right)=\frac{(c-b)_n}{(c)_n}\,{}_2F_1\left(\begin{matrix} -n,b \\ b-n+1-c \end{matrix};1-x\right),\qquad n=0,1,\ldots. $$

The first contains a number of examples Euler gave of transformations of series that speed convergence. For example, when $x=-1$, the series ${}_2F_1\left(\begin{matrix} a,b \\ c \end{matrix};-1\right)$ converges slowly, whereas ${}_2F_1\left(\begin{matrix} a,c-b \\ c \end{matrix};\frac{1}{2}\right)$ converges much more rapidly. In an age when computation is easy and relatively inexpensive, we find it hard to realize how many mathematical developments were stimulated by the desire to compute something. These transformation formulas, along with Euler's transformation, were the first of a limited number of transformation formulas between generalized hypergeometric series which have been discovered in the last two hundred years. Another one is Regge's symmetry of the $3-j$ symbols mentioned earlier. Gauss found the correct extension of Pfaff's second transformation in the case when the series does not terminate. The factor

$$ \frac{(c-b)_n}{(c)_n}=\frac{\Gamma(n+c-b)\Gamma(c)}{\Gamma(n+c)\Gamma(c-b)} $$

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becomes

$$\frac{\Gamma(c-a-b)\Gamma(c)}{\Gamma(c-a)\Gamma(c-b)}$$

when $-n$ is replaced by a, as one might suspect, but that is not the only change. There is another term that must be added.

Gauss also considered a different type of result. He defined two hypergeometric series to be contiguous if all their parameters are the same with one exception, and if they differ by one in this parameter. He showed that a general ${}_2F_1\left(\begin{matrix}a,b\\c\end{matrix};x\right)$ and any two ${}_2F_1$ series that are contiguous to it are linearly dependent. There are nine such relations after the symmetry of ${}_2F_1\left(\begin{matrix}a,b\\c\end{matrix};x\right)$ in a and b is used. These contiguous relations can be iterated, so any three functions ${}_2F_1\left(\begin{matrix}a+j,b+k\\c+l\end{matrix};x\right)$ with j,k,l integers are linearly dependent. Since

$$\frac{d}{dx}\,{}_2F_1\left(\begin{matrix}a,b\\c\end{matrix};x\right)=\frac{ab}{c}\,{}_2F_1\left(\begin{matrix}a+1,b+1\\c+1\end{matrix};x\right),$$

it is easy to see that Euler's differential equation for ${}_2F_1\left(\begin{matrix}a,b\\c\end{matrix};x\right)$ can be written as one of these iterated contiguous relations. At the end of his one published paper on hypergeometric series, Gauss stated this difference equation. His second paper, which remained unpublished during his life, treated this equation as a differential equation and he found most of the explicit formulas that can be derived directly from this equation. This includes the quadratic transformations, which play a fundamental role in a number of problems. To get a better perspective on these transformations, two other important eighteenth-century discoveries need to be considered.

One was the study of elliptic integrals by Fagnano, Euler, Landen, and Legendre, and of the arithmetic-geometric mean by Lagrange and Gauss. The other was the introduction of spherical harmonics and Legendre polynomials by Legendre and Laplace. The first of these developments led to elliptic functions, a subject that was studied extensively in the last three quarters of the nineteenth century by Abel, Jacobi, Eisenstein, Weierstrass, Hermite, and many others. The second is directly tied up with some of the algebraic approaches to special functions which have been developed in the last fifty years. A good historical summary of the early work on elliptic integrals was given by Mittag-Leffler (see [6]); Landen's transformation in the form given by Lagrange is described there (the reference to Enneper on page 291 should be to page 357, not page 307). Gauss's quadratic transformation of the elliptic integral of the first type is also given by Mittag-Leffler. Lagrange was motivated by a desire to compute the value of an

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important integral. Gauss first considered the sequences $a_{n+1}=(a_n+b_n)/2$, $b_{n+1}=(a_nb_n)^{1/2}$; observed that they converge, and was able to recognize the value they converge to when $a_0=2^{1/2}$, $b_0=1$; and finally evaluated the limit in general. Gauss then used this result to lead him to two further results, the introduction of the lemniscate functions, which are special elliptic functions, and of the two general quadratic transformations of the ordinary hypergeometric function ${}_2F_1(a,b;c;x)$ with different restrictions on one of the parameters. These functions form a very important subclass of the general ${}_2F_1$, for after they have been multiplied by an appropriate algebraic function, they are exactly the class of hypergeometric series that we call Legendre functions.

Legendre polynomials were studied extensively by Legendre and Laplace in the 1780s. They can be introduced in the following way. The function $(c^2-2cr\cos\theta+r^2)^{-1/2}$ represents the potential in an inverse square field at a point P of a source at C, where r and c are the distances from P and C to a fixed point O, and θ is the angle between the segments PO and OC. This function can be expanded in a power series in r to give

$$(c^2-2cr\cos\theta+r^2)^{-1/2}=\sum_{n=0}^{\infty} P_n(\cos\theta)r^nc^{-n-1}.$$

$P_n(x)$ is a polynomial of degree n in x which we call the Legendre polynomial. Legendre and Laplace discovered the following facts about these polynomials.

$$\int_{-1}^{1} P_n(x)P_m(x)\,dx=0,\quad m\neq n;\qquad \int_{-1}^{1}(P_n(x))^2\,dx=\frac{2}{2n+1}. \tag{L.1}$$

$$\begin{aligned}&\int_0^{\pi} P_n(\cos\theta)P_m(\cos\theta)\sin\theta\,d\theta=0,\qquad m\neq n;\\ &\int_0^{\pi}[P_n(\cos\theta)]^2\sin\theta\,d\theta=\frac{2}{2n+1}.\end{aligned} \tag{L.1a}$$

$$P_n(\cos\theta)=(1/\pi)\int_0^{\pi}[\cos\theta+i\sin\theta\cos\varphi]^n\,d\varphi. \tag{L.2}$$

$$P_n(\cos\theta)P_n(\cos\varphi)=(1/\pi)\int_0^{\pi}P_n(\cos\theta\cos\varphi+\sin\theta\sin\varphi\cos\Psi)\,d\Psi. \tag{L.3}$$

$$(1-x^2)y''-2xy'+n(n+1)y=0,\qquad y=P_n(x). \tag{L.4}$$

$$\begin{aligned}P_n(\cos\theta\cos\varphi+\sin\theta\sin\varphi\cos\Psi)&=P_n(\cos\theta)P_n(\cos\varphi)\\ &+2\sum_{k=1}^{n}\frac{(n-k)!}{(n+k)!}P_n^k(\cos\theta)P_n^k(\cos\varphi)\cos k\Psi.\end{aligned} \tag{L.5}$$

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The associated Legendre functions are defined by

$$P_n^k(x)=(-1)^k(1-x^2)^{k/2}\frac{d^k}{dx^k}P_n(x), \qquad -1<x<1,\ k=1,\dots,n. \tag{L.6}$$

Earlier Lagrange had come across these same polynomials as solutions to a difference equation

$$(2n+1)xP_n(x)=(n+1)P_{n+1}(x)+nP_{n-1}(x). \tag{L.7}$$

Each of the foregoing results is only one of an extensive class of formulas for more general special functions. To see what they are, the corresponding results for trigonometric functions will be given next and then a description of the natural setting for these formulas will be given. Since $\cos n\theta$ is a polynomial of degree n in $\cos\theta$, we will consider $T_n(x)$, which is defined by $T_n(\cos\theta)=\cos n\theta$.

$$\begin{aligned}&\int_{-1}^{1}T_n(x)T_m(x)(1-x^2)^{-1/2}dx=0, \qquad m\neq n,\\ &\int_{-1}^{1}[T_n(x)]^2(1-x^2)^{-1/2}dx=\begin{cases}\pi, & n=0,\\ \dfrac{\pi}{2}, & n=1,2,\dots.\end{cases}\end{aligned} \tag{T.1}$$

$$\begin{aligned}&\int_0^\pi \cos n\theta\cos m\theta\, d\theta=0, \qquad m\neq n,\\ &\int_0^\pi \cos^2 n\theta\, d\theta=\begin{cases}\pi, & n=0,\\ \dfrac{\pi}{2}, & n=1,2,\dots.\end{cases}\end{aligned} \tag{T.1a}$$

$$\cos n\theta=\frac{e^{in\theta}+e^{-in\theta}}{2}. \tag{T.2}$$

$$\cos n\theta\cos n\varphi=\frac{1}{2}\left[\cos n(\theta+\varphi)+\cos n(\theta-\varphi)\right]. \tag{T.3}$$

$$(1-x^2)y''-xy'+n^2y=0, \qquad y=T_n(x). \tag{T.4}$$

$$u''(\theta)+n^2u(\theta)=0, \qquad u=\cos n\theta. \tag{T.4a}$$

$$\cos n(\theta+\varphi)=\cos n\theta\cos n\varphi-\sin n\theta\sin n\varphi. \tag{T.5}$$

$$\begin{aligned}&\frac{d\cos n\theta}{d\theta}=-n\sin n\theta,\\ &\frac{d\cos n\theta}{d\cos\theta}=\frac{dT_n(x)}{dx}=\frac{n\sin n\theta}{\sin\theta}=nU_{n-1}(x), \qquad x=\cos\theta.\end{aligned} \tag{T.6}$$

$$2\cos\theta\cos n\theta=\cos(n+1)\theta+\cos(n-1)\theta; \tag{T.7}$$

$$\begin{aligned}&xT_n(x)=\tfrac{1}{2}T_{n+1}(x)+\tfrac{1}{2}T_{n-1}(x), \qquad n=1,2,\dots,\\ &xT_0(x)=T_1(x).\end{aligned} \tag{T.7a}$$

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The orthogonality relations (L.1) and (T.1) are fundamental. Since both $P_n(x)$ and $T_n(x)$ are polynomials, they are orthogonal polynomials. Any set of polynomials in one variable that is orthogonal with respect to a positive measure satisfies a three-term recurrence relation

$$xp_n(x) = A_n p_{n+1}(x) + B_n p_n(X) + C_n p_{n-1}(x)$$

with $A_{n-1}C_n > 0$, B_n real. Conversely, any set of polynomials that satisfy this recurrence relation are orthogonal with respect to a positive measure when $A_{n-1}C_n > 0$ and B_n is real. If $A_{n-1}C_n > 0$, $(n = 1, 2, \ldots, N)$, $A_N C_{N+1} = 0$, then the polynomials are orthogonal with respect to a positive measure that has only finitely many points of support. This recurrence relation reminds one of Gauss's contiguous relations for ${}_2F_1$'s, and there are a number of cases when the recurrence relation can be shown to be an instance of one of Gauss's formulas or an iterate of these formulas. In other cases there are other hypergeometric series, either ${}_3F_2\left(\begin{matrix} a,b,c \\ d,e \end{matrix}; 1\right)$ or ${}_4F_3\left(\begin{matrix} -n, n+a, b, c \\ d, e, f \end{matrix}; 1\right)$ where $a+b+c+1 = d+e+f$, which satisfy more general contiguous relations that lead to orthogonal polynomials. Now the polynomial variable is in one or more of the parameter spots, rather than a power series variable. As a result of this and our too exclusive interest in power series, these polynomials were not studied and applied as early and as often as they should have been.

One of the reasons $\cos\theta$ and $\sin\theta$ are so useful is their connection with the circle. The addition formula (T.5) is most easily proved by using a rotation of the circle. Cauchy gave this proof. Similarly, the addition formula for $P_n(x)$, which is (L.5), arose by considering the rotation group acting on the sphere in R^3.

To understand the setting, consider first the circle. A function $f(\theta)$, $0 \leqslant \theta \leqslant 2\pi$, $f(0) = f(2\pi)$, can be expanded in a Fourier series

$$f(\theta) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta)$$

where

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\theta)\cos n\theta\, d\theta, \qquad b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\theta)\sin n\theta\, d\theta.$$

One application of this expansion is to the construction of a harmonic function $u(x,y)$ for $x^2 + y^2 < 1$, which assumes a given boundary value. For let

$$u(x,y) = \frac{a_0}{2} + \sum_{n=1}^{\infty} r^n [a_n \cos n\theta + b_n \sin n\theta],$$

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$x=r\cos\theta$, $y=r\sin\theta$. Then $u(x,y)$ is harmonic; that is,

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=0$$

and

$$\lim_{r\to 1^-} u(r\cos\theta, r\sin\theta)=f(\theta)$$

when $f(\theta)$ is continuous for $0\leqslant\theta\leqslant 2\pi$.

A similar problem exists for three variables, and it is solved in a similar way. First, one must find a set of functions that satisfies Laplace's equation

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}=0$$

for $x^2+y^2+z^2<1$. This is done by introducing spherical coordinates $x=r\cos\varphi\sin\theta$, $y=r\sin\varphi\sin\theta$, $z=r\cos\theta$, $0\leqslant\varphi\leqslant 2\pi$, $0\leqslant\theta\leqslant\pi$, and finding solutions of Laplace's equation of the form $a(r)b(\theta)c(\varphi)$. One can take $a(r)=r^n$, $c(\varphi)=\cos k\varphi$ or $\sin k\varphi$, and then $b(\theta)$ can be taken to be $P_n^k(\cos\theta)$. The functions $r^n\cos n\theta=\mathrm{Re}(x+iy)^n$ and $r^n\sin n\theta=\mathrm{Im}(x+iy)^n$ are homogeneous polynomials of degree n in x and y. Similarly, $r^nP_n^k(\cos\theta)\cos k\varphi$ and $r^nP_n^k(\cos\theta)\sin k\varphi$, $k=0,1,\ldots,n$, are homogeneous harmonic polynomials of degree n in x, y, and z which are linearly independent. There are $2n+1$ of these, and this is the same number that appears the denominator in (L.1). Similarly, the functions $r^n\cos n\theta$ and $r^n\sin n\theta$ are linearly independent when $n=1,2,\ldots$, and there are two of them, while for $n=0$ there is only one. This explains the denominators in (T.1). These homogeneous harmonic polynomials are then used to construct a harmonic function for $x^2+y^2+z^2<1$ with given boundary values in exactly the same way as in the case of the circle, since the functions $P_n^k(\cos\theta)\cos k\varphi$ and $P_n^k(\cos\theta)\sin k\varphi$, $k=0,1,\ldots,n$, $n=0,1,\ldots$, form a complete orthogonal set of functions.

Formula (L.3) is the basic functional equation satisfied by the zonal spherical harmonic of degree n on S^2. Zonal means independence from the angle φ. We call the zonal spherical harmonics spherical functions. The general setting for such spherical functions is a space with a distance function and a group G operating on this space. The space is homogeneous in that any point can be mapped to any other point by the group. Also, the space should have the property that if $d(x_1,y_1)=d(x_2,y_2)$, then there is $g\in G$ with $g(x_1)=x_2$, $g(y_1)=y_2$. Such spaces are said to be two-point homogeneous. In addition to the sphere in R^3, spheres of any dimension, projective spaces over the reals, complexes, and quaternions, and a two-dimensional projective space over the Cayley numbers are compact two-point homogeneous spaces which are Riemannian manifolds. In each of

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these cases the spherical functions are orthogonal polynomials in a variable depending on the distance. Each of these orthogonal polynomials is also a hypergeometric function of the type ${}_2F_1\left(\begin{matrix}-n, n+a\\ b\end{matrix}; t\right)$ for some a and b. The measure $\sin\theta\, d\theta$ in the case (L.1a) comes from looking at the size of an orbit of a small arc $d\theta$ under a rotation that leaves the north pole fixed.

There are other very important two-point homogeneous spaces which are compact. The easiest to visualize is the set of vertices of the unit cube in R^N. Again the spherical functions are orthogonal polynomials, and they are orthogonal with respect to the symmetric binomial distribution $\binom{N}{x}2^{-N}$, $x = 0, 1, \ldots, N$, since this is the size of the orbit of any point with x zeros and $N-x$ ones under the octahedral group acting on this space and leaving $(0, 0, \ldots, 0)$ fixed. These orthogonal polynomials are also hypergeometric functions, ${}_2F_1\left(\begin{matrix}-n, -x\\ -N\end{matrix}; 2\right)$, x, $n = 0, 1, \ldots, N$, and their three-term recurrence relation is one of the Gauss contiguous relations. They are called Krawtchouk polynomials, though they were introduced almost one hundred years ago by Gram, and they play an important role in coding theory, a subject covered in Volume 3 (*The Theory of Information and Coding*) in this Encyclopedia.

The differential equations (L.4) and (T.4), (T.4a) arise when Laplace's equation is solved by separation of variables. The addition formulas (L.5) and (T.5) are among the most important facts known about these functions. In most of the cases of two-point homogeneous spaces where explicit formulas have been found for the spherical functions there is an addition formula that contains the functional equation as the constant term in an orthogonal expansion. For example, if (L.5) is integrated on $[0, \pi]$ with respect to $d\Psi$ and (T.1a) is used, the result is (L.3). The most natural way to derive addition formulas of this type is to use a group acting on the space, and this is essentially the method used by Laplace and Legendre almost two hundred years ago.

Another important class of functions that were introduced in the eighteenth century are Bessel functions. The Bessel function of the first kind $J_\alpha(x)$ can be defined by

$$J_\alpha(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (x/2)^{2n+\alpha}}{\Gamma(n+\alpha+1)n!} = \frac{(x/2)^\alpha}{\Gamma(\alpha+1)}\,{}_0F_1\left(\begin{matrix}-\\ \alpha+1\end{matrix}; \frac{-x^2}{4}\right).$$

After the elementary transcendental functions, these are the class that have been studied most extensively and they have been used in many fields where mathematics has been applied. They have a strong connection with Legendre functions which has been studied by many people. A simple example is Mehler's formula

$$\lim_{n\to\infty} P_n\left(\cos\frac{z}{n}\right) = J_0(z).$$

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This can be interpreted by considering Legendre polynomials as spherical functions on a sphere of large radius and seeing what happens in a neighborhood of the north pole. The sphere becomes flat and this suggests that $J_0(z)$ should play a role in R^2 similar to that of $P_n(\cos\theta)$ on S^2. The analogues of zonal functions are called radial functions, those functions which depend only on the distance from the origin. One important fact is due to Poisson. If $f(x_1,x_2)=g((x_1^2+x_2^2)^{1/2})$ and

$$F(y_1,y_2)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x_1,x_2)\exp\left[i(x_1y_1+x_2y_2)\right]dx_1\,dx_2,$$

then

$$F(y_1,y_2)=G\left(\left(y_1^2+y_2^2\right)^{1/2}\right)$$

and

$$G(t)=2\pi\int_0^{\infty} g(r)rJ_0(rt)\,dr.$$

The next big development in special functions was the introduction of elliptic functions and theta functions by Abel and Jacobi. Again Mittag-Leffler's paper gives a good historical summary. There have been a few other developments since then that allow us to view the subject with a slightly different perspective. One important development was when Heine introduced what are now called basic hypergeometric series. Recall that a hypergeometric series is a series Σa_n with a_{n+1}/a_n a rational function of n. A basic hypergeometric series is a series Σa_n with a_{n+1}/a_n a rational function of q^n for some fixed q. The role played by the shifted factorial $(a)_n$ in hypergeometric series is now played by $(a;q)_n=(1-a)(1-aq)\cdots(1-aq^{n-1})$. If $|q|<1$, then $(a;q)_\infty=\prod_{n=0}^{\infty}(1-aq^n)$ and $(a;q)_n=(a;q)_\infty/(aq^n;q)_\infty$ is defined for noninteger values of n as long as $aq^{n+k}\neq 1$, $k=0,1,\ldots$. Euler had evaluated two basic hypergeometric series:

$$\sum_{n=0}^{\infty}\frac{x^n}{(q;q)_n}=\frac{1}{(x;q)_\infty};\qquad \sum_{n=0}^{\infty}(-1)^n\frac{q^{\binom{n}{2}}x^n}{(q;q)_n}=(x;q)_\infty.$$

These are special cases of the q-binomial theorem

$$\sum_{n=0}^{\infty}\frac{(a;q)_n}{(q;q)_n}x^n=\frac{(ax;q)_\infty}{(x;q)_\infty},$$

a result which is attributed to many different people. Heine discovered it when he introduced the basic analogue of ${}_2F_1\left(\begin{matrix}a,b\\c\end{matrix};x\right)$ in 1847. Cauchy

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had published a proof a few years before this, and Jacobi gave a reference to an 1820 book of Schweins. This formula is given by Schweins, but he refers to an earlier work of Rothe. Unfortunately I have not seen Rothe's book and so cannot confirm the 1811 date given by Schweins. However, it seems very likely that he is correct. Gauss published related formulas in 1811.

One of the most important basic hypergeometric series is the theta function

$$\sum_{-\infty}^{\infty} q^{n^2}x^n=(q^2;q^2)_\infty(-qx;q^2)_\infty(-qx^{-1};q^2)_\infty.$$

This was not the first instance of a bilateral series (one which is infinite in both directions), for

$$\begin{aligned}\pi\cot\pi z &= \lim_{n\to\infty}\sum_{m=-n}^{n}\frac{1}{z-m}\\ &= \sum_{m=-\infty}^{\infty}\left(\frac{1}{z-m}-\frac{1}{\frac{1}{2}-m}\right)=\sum_{-\infty}^{\infty}\frac{\left(\frac{1}{2}-z\right)}{(m-z)\left(m-\frac{1}{2}\right)}\end{aligned}$$

and

$$\frac{\pi^2}{(\sin\pi z)^2}=\sum_{n=-\infty}^{\infty}\frac{1}{(z-n)^2}.$$

However, it was a very fruitful discovery. Initially Jacobi, in his treatment of elliptic functions in *Fundamenta Nova Theoriae Functionum Ellipticarum*, 1829, derived results about theta functions as consequences of results on elliptic functions. Later he reversed this procedure and used theta functions to derive facts about elliptic functions. The function $\sum_{-\infty}^{\infty} q^{n^2}x^n$ had occurred in Fourier's work on the heat equation, and Poisson derived a very important transformation of this function, but the realization that this function was fundamental is due to Jacobi. Recently a new setting for this function has been discovered which ties it up with a group-theoretic approach similar to that outlined above. The relevant group is the three-dimensional Heisenberg group, the group of matrices

$$\begin{bmatrix}1 & z & y\\ 0 & 1 & x\\ 0 & 0 & 1\end{bmatrix}.$$

(See Cartier [3] and Auslander and Tolimieri [1].) Other basic hypergeometric series are orthogonal polynomials that arise as spherical functions

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on discrete two-point homogeneous spaces with certain Chevalley groups acting on these spaces. It is too early in the development of these ideas to say how important they will be, but I am reasonably sure that some important results will be obtained from them. In the nineteenth century elliptic functions were studied exhaustively and they seemed to have a secure place in the mathematics curriculum. Many ideas arose out of scholars' efforts to understand them. However, they themselves have not been as useful as one would have hoped, and as a result their place in the standard curriculum was taken by other subjects that were thought to be more useful, and for decades the knowledge of elliptic functions was largely restricted to number theorists and some applied mathematicians and engineers. Now many people who study and use combinatorial arguments are going to have to learn something about basic hypergeometric series. This will include statisticians interested in block designs and many people studying and using computer algorithms. They play a central role in the study of partitions, the subject of Volume 2 (*The Theory of Partitions*) in this Encyclopedia.

Another development in the study of special functions in the last century was the introduction of differential equations with more than three regular singular points. Riemann observed that Euler's differential equation

$$x(1-x)y''+[c-(a+b+1)x]y'-aby=0, \qquad y={}_2F_1\left(\begin{matrix}a,b\\c\end{matrix};x\right),$$

has regular singular points at $x=0$, 1, ∞, and by a linear fractional transformation these singular points can be put at three arbitrary points. The resulting differential equation is determined by the location of these singularities and certain parameters which determine the nature of the solutions in neighborhoods of the singular points. He showed how to obtain the results of Gauss, Kummer, and some of Jacobi's work on hypergeometric series in a simple way and found a cubic transformation which is still not really understood. However, the real importance of this work was the realization that the singularities of a differential equation determine much more about the solutions than one would have thought. Other differential equations were introduced; Heun, Mathieu, Lamé, and those for spheroidal wave functions are examples. These often arose when the wave equation or Laplace's equation was reduced to ordinary differential equations by separating variables. The solutions to these equations give interesting special functions which are much more complicated than hypergeometric functions. It is still not clear how best to study these functions, and one hopes that the algebraic methods used by Miller in this book will allow us to really understand these important functions.

Appell introduced hypergeometric functions of two variables and found analogues of some of the useful facts about the ordinary hypergeometric function for them. However, a real understanding of hypergeometric

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functions in two variables still lies in the future, though we now have a few ways of treating parts of this subject that have been fruitful.

Pincherle, and later Mellin and Barnes, introduced a new way of treating hypergeometric series and functions. They integrated quotients of gamma functions and were able to perform analytic continuations with ease. The type of integrals they considered has arisen in many different places, from Mehler's earlier work on electrical problems with conical symmetry to Bargmann's work on representations of the Lorentz group.

Poincaré discovered an important extension of elliptic functions when he introduced automorphic functions. They have been extended to several variables in a number of ways. One of the most fruitful is due to Siegel and involves functions of matrix argument. Matrix argument gamma functions were introduced somewhat earlier by Ingham, who was led to them by work of statisticians. In terms of the special functions that are useful in applied mathematics, the main usefulness of automorphic functions will probably be the methods that were used to develop a theory in several variables; for although the theory of hypergeometric and basic hypergeometric functions in several variables is largely undeveloped, enough results have been obtained to indicate that many deep results can be found. A recent example is the work of Macdonald on identities similar to the triple product for the theta function, which he derived from affine root systems of the classical Lie algebras. Feynman integrals can be considered as multivariate hypergeometric functions [4], as are the $3n-j$ symbols which are used to decompose tensor products of representations of $SU(2)$ [2]. Both of these are very useful, yet far from understood. So this area of mathematics is no different than most other parts of mathematics; the pressing problems are to understand what happens in several variables.

One term which has not been defined so far is "special function." My definition is simple, but not time invariant. A function is a special function if it occurs often enough so that it gets a name. There are a number of very important special functions which do not fit into the framework outlined earlier—for example, the Riemann zeta function, which plays a central role in the study of primes and many other number-theoretic problems. Other examples are the Bernoulli polynomials and Bernoulli numbers. Bernoulli numbers were introduced to aid in the computation of series, and they now appear in many unexpected places.

Harry Bateman had a list of over a thousand special functions. Although many of these were special hypergeometric series with no reason for having a separate name, since everything that was known about them was a special case of facts known about a more general hypergeometric series, there are clearly too many functions to make it worthwhile to write books on each of them. However, some of them have so many interesting properties and occur so often that it is essential that each generation of mathematicians consider them anew and record their results for others to

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use. It is too early to say exactly what books on special functions will appear in this series, but at present there is no adequate treatment of hypergeometric and basic hypergeometric series. There are a few books that treat special functions from an algebraic point of view [5, 7, 8], but none of these contain the very interesting work on the unitary group which led to addition formulas for Jacobi and Laguerre polynomials and for the disk polynomials, an important class of orthogonal polynomials in two variables. The discrete orthogonal polynomials have also not been treated in an adequate way. Books on all these topics will be written.

There have also been some very interesting applications of special functions to combinatorial problems that have only partially been treated in previously mentioned Volumes 2 and 3 in this Encyclopedia. Beyond this we will have to wait and see what develops. If experience is a guide, we will be surprised by the next development. Such developments are predictable in retrospect, but not before the fact.

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Cambridge University Press
978-0-521-17739-9 - Symmetry and Separation of Variables: Encyclopedia of Mathematics and its Applications: Volume 4
Willard Miller
Frontmatter
More information

Preface

This book is concerned with the relationship between symmetries of a linear second-order partial differential equation of mathematical physics, the coordinate systems in which the equation admits solutions via separation of variables, and the properties of the special functions that arise in this manner. It is an introduction intended for anyone with experience in partial differential equations, special functions, or Lie group theory, such as group theorists, applied mathematicians, theoretical physicists and chemists, and electrical engineers. We will exhibit some modern group-theoretic twists in the ancient method of separation of variables that can be used to provide a foundation for much of special function theory. In particular, we will show explicitly that all special functions that arise via separation of variables in the equations of mathematical physics can be studied using group theory. These include the functions of Lamé, Ince, Mathieu, and others, as well as those of hypergeometric type.

This is a very critical time in the history of group-theoretic methods in special function theory. The basic relations between Lie groups, special functions, and the method of separation of variables have recently been clarified. One can now construct a group-theoretic machine that, when applied to a given differential equation of mathematical physics, describes in a rational manner the possible coordinate systems in which the equation admits solutions via separation of variables and the various expansion theorems relating the separable (special function) solutions in distinct coordinate systems. Indeed for the most important linear equations, the separated solutions are characterized as common eigenfunctions of sets of second-order commuting elements in the universal enveloping algebra of the Lie symmetry algebra corresponding to the equation. The problem of expanding one set of separable solutions in terms of another reduces to a problem in the representation theory of the Lie symmetry algebra.

Although this method is simple, elegant, and very useful, it has as yet been applied to relatively few differential equations. (At the time of this writing, the wave equation $(\partial_{tt}-\Delta_3)\Psi=0$ is still under intensive study.) Moreover, few theorems have yet been proved that delineate the full scope of the method. It is the author's hope that the present work, which is aimed at a general audience rather than at specialists, will convince the reader that group-theoretic methods are singularly appropriate for the study of separation of variables and special functions. It is also hoped that this work will encourage others to enter the field and solve the many interesting problems that remain.

The ideas relating Lie groups, special functions, and separation of variables spring from a number of rather diverse historical sources. The first deep work on the relationship of group representation theory and special functions is commonly attributed to E. Cartan (27). However, the first detailed use of the relationship for computational purposes is probably found in the papers of Wigner. Wigner's work on this subject began in the 1930s and is given an elementary exposition in his 1955 Princeton lecture notes. These notes were later expanded and updated in a book by Talman (124).

A second major contributor to the computational theory is Vilenkin, who wrote a series of papers commencing in 1956 and culminating in his book (128). This encyclopedic treatise was strongly influenced by the explicit constructions of irreducible representations of the classical groups due to Gel'fand and Naimark (e.g., (41)). Vilenkin (and Wigner) obtain special functions as matrix elements of operators defining irreducible group representations.

Another precursor of our theory is the factorization method. The method was discovered by Schrödinger and applied to solve the time-independent Schrödinger equation for a number of systems of physical interest (e.g., (117)). This useful tool for computing eigenvalues and recurrence relations for solutions of second-order ordinary differential equations was developed by several authors, including Infeld and Hull (52), who summarized the state of the theory as of 1951. An independent and somewhat different development was given by Inoui (53).

The author contributed to this theory by showing, in 1964 (80), that the factorization method was equivalent to the representation theory of four Lie algebras.

Another approach to the subject matter of this book is contained in three remarkable papers by Weisner (133–135), the first appearing in 1955. Weisner showed the group-theoretic significance of families of generating functions for hypergeometric, Hermite, and Bessel functions. In these papers are also found examples of separable coordinate systems characterized in terms of Lie algebra symmetry operators. Weisner's theory is extended and related to the factorization method in the author's monograph (82). This monograph is primarily devoted to the representation theory of local Lie groups rather than the theory of global Lie groups, which is treated in the works of Talman and Vilenkin.

We should also mention Truesdell's monograph on the F equation (126), which demonstrated how generating functions and integral representations for special functions can be derived directly from a knowledge of the differential recurrence relations obeyed by the special functions. By 1968 it was recognized that Truesdell's technique fits comfortably into the group-theoretic approach to special functions (82).

A major theme in the present work is that separable coordinate systems for second-order linear partial differential equations can be characterized in terms of sets of second-order symmetry operators for the equations. This idea is very natural from a quantum-mechanical point of view. Moreover, since the work of Lie, it has been known to be correct for certain simple coordinates, such as spherical, cylindrical, and Cartesian (i.e., subgroup) coordinates. For a few important Schrödinger equations, such as the equation for the hydrogen atom, operator characterizations of a few nonsubgroup coordinates were well known (9, 30). However, the explicit statement of the relationship between symmetry and separation of variables appeared for the first time in the 1965 paper (138) by Winternitz and Fris. These authors gave group-theoretic characterizations of the separable coordinate systems corresponding to the eigenvalue equations for the Laplace-Beltrami operators on two-dimensional spaces with constant curvature. This work was extended by Winternitz and collaborators in (74, 106, 139, 140). Finally, the author in collaboration with C. P. Boyer and E. G. Kalnins has classified group theoretically the separable coordinate systems for a number of important partial differential equations and investigated the relationship between the classification and special function theory. One interesting feature of this work, primarily due to Kalnins, has been the discovery of many new separable systems that are not contained in such standard references as (97). A second feature has been the development of a group-theoretic method that makes it possible to derive identities for nonhypergeometric special functions, such as Mathieu, Lamé, spheroidal, Ince, and anharmonic oscillator functions, as well as for the more familiar hypergeometric functions.

Prerequisites for understanding this book include some acquaintance with Lie groups and algebras (i.e., homomorphism and isomorphism of groups and algebras) such as can be found in (43) and (85). However, the examples treated here are very explicit and can be understood with only a minimal knowledge of Lie theory. Secondly, it is assumed that the reader has some experience in the solution of partial differential equations by separation of variables, in, say, rectangular, polar, and spherical coordinates.

Due to limitations of space, time, and the author's competence, it has been found necessary to omit certain topics. The most important among these is the theory of spherical functions on groups. This topic, a generalization of the theory of spherical harmonics, has an extensive literature (e.g., [47, 130]). Moreover, spherical functions were recently used to derive an addition theorem for Jacobi polynomials (68, 119). However, spherical functions are always associated with subgroup coordinates, and even for the most elementary equations considered in this book, they fail to encompass all of the special functions that arise via separation of variables.

Boundary value problems have also been omitted, even though symmetry methods are important for their solution (see [16]). This last reference, as well as (105) and (38) contain discussions of symmetry techniques for finding solutions of nonlinear partial differential equations, a subject that has been omitted here because its ultimate forum is not yet clear.

I should like to thank Paul Winternitz for helpful discussions leading to the basic concepts relating symmetry and separation of variables. Finally, I wish to thank Charles Boyer and Ernie Kalnins, without whose research collaboration this book could not have been written.

WILLARD MILLER, JR.