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Special orthogonal polynomials in quantum mechanics

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Abstract: Using an algebraic method for solving the wave equation in quantum mechanics, we encountered a new class of orthogonal polynomials on the real line. One of these is a four-parameter polynomial with a discrete spectrum. Another that appeared while solving a Heun-type equation has a mix of continuous and discrete spectra. Based on these results and on our recent study of the solution space of an ordinary differential equation of the second kind with four singular points, we introduce a modification of the hypergeometric polynomials in the Askey scheme. Up to now, all of these polynomials are defined only by their three-term recursion relations and initial values. However, their other properties like the weight function, generating function, orthogonality, Rodrigues-type formula, etc. are yet to be derived analytically. This is an open problem in orthogonal polynomials.

Keywords: tridiagonal representation; orthogonal polynomials; potential functions; asymptotics; recursion relation; spectrum formula

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1. Introduction

The wave function in quantum mechanics could be viewed as a vector field in an infinite dimensional space with local unit vectors. Therefore, in one of the formulations of quantum mechanics, the wave function at an energy *E*, $|\psi_E(x)\rangle$, is written as a bounded sum over a complete set of square integrable basis functions in configuration space with coordinate *x*:

$$|\psi_E(x)\rangle = \sum_n f_n(E)|\phi_n(x)\rangle, \qquad (1)$$

where $\{\phi_n(x)\}$ are the basis elements (local unit vectors) and $\{f_n(E)\}$ are proper expansion coefficients in the energy (the components of the wave function along the unit vectors). All physical information about the system, both structural and dynamical, are contained in these expansion coefficients. The "*Tridiagonal Representation Approach* (TRA)" is an algebraic method for solving the wave equation (e.g., the Schrödinger or Dirac equation) [1-4]. In the TRA, the basis elements are chosen such that the matrix representation of the wave operator is tridiagonal. Consequently, the resulting matrix wave equation becomes a three-term recursion relation for the expansion coefficients $\{f_n(E)\}$, which is solved in terms of orthogonal polynomials in some physical parameter(s) and/or the energy. If we write $f_n(E) = f_0(E)P_n(\varepsilon)$, where ε is an appropriate function of the energy and physical parameters, then we have shown that $\{P_n(\varepsilon)\}$ is a complete set of orthogonal polynomials satisfying the said recursion relation with $P_0(\varepsilon) = 1$. The corresponding positive definite weight function is $[f_0(E)]^2$. These polynomials are associated with the continuum scattering states of the system where *E* is a continuous set. On the other hand, the discrete bound states are associated with the discrete version of these polynomials.

We found all such polynomials that correspond to well-known physical systems and to new ones as well. For example, the scattering states of the Coulomb problem are associated with Meixner-Pollaczek polynomial whereas the bound states are associated with one of its discrete versions; the

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Meixner polynomial. Moreover, the scattering states of the Morse oscillator are associated with the continuous dual Hahn polynomial whereas the finite number of bound states are associated with its discrete version, the dual Hahn polynomial. Additionally, the continuum scattering states of the hyperbolic Pöschl-Teller potential correspond to the Wilson polynomial whereas the finite number of bound states are associated with the Racah polynomial, which is the discrete version of the Wilson polynomial. And so on.

On the other hand, since 2005 and while using the TRA we have been frequently faced with members of a new class of exactly solvable problems that are associated with orthogonal polynomials, which were overlooked in the mathematics and physics literature [5-12]. These polynomials are defined, up to now, by their three-term recursion relations and initial value $P_0(\varepsilon)=1$. However, their other important properties are yet to be derived analytically. These properties include the weight functions, generating functions, asymptotics, orthogonality relations, Rodrigues-type formulas, etc. Due to the prime significance of these polynomials in physics and mathematics, we call upon experts in the field of orthogonal polynomials to study them, derive their properties and write them in closed form (e.g., in terms of the hypergeometric functions). Two of these polynomials are defined in sections 2 and 3 whereas in section 4 we introduce a modification to the hypergeometric polynomials in the Askey scheme [13,14] that manifest itself in a particular deformation of their three-term recursion relations.

2. The first polynomial

The four-parameter orthogonal polynomial, which we designate as $H_n^{(\mu,\nu)}(z;\alpha,\theta)$, satisfies the following three-term recursion relation.

$$\begin{aligned}(\cos\theta)H_n^{(\mu,\nu)}(z;\alpha,\theta)=&\left\{z\sin\theta\left[\left(n+\tfrac{\mu+\nu+1}{2}\right)^2-\alpha^2\right]+\tfrac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\right\}H_n^{(\mu,\nu)}(z;\alpha,\theta)\\&+\tfrac{2(n+\mu)(n+\nu)}{(2n+\mu+\nu)(2n+\mu+\nu+1)}H_{n-1}^{(\mu,\nu)}(z;\alpha,\theta)+\tfrac{2(n+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+2)}H_{n+1}^{(\mu,\nu)}(z;\alpha,\theta)\end{aligned} \quad (2)$$

where $z\in\mathbb{R}$, $0<\theta\le\pi$ and $n=1,2,\ldots$. It is a polynomial of degree n in z. Setting $z\equiv 0$ turns (2) into the recursion relation of the Jacobi polynomial $P_n^{(\mu,\nu)}(\cos\theta)$. Physical requirements dictate that μ and ν are greater than −1. The polynomial of the first kind satisfies this recursion relation together with $H_0^{(\mu,\nu)}(z;\alpha,\theta)=1$ and

$$H_1^{(\mu,\nu)}(z;\alpha,\theta)=\frac{\mu-\nu}{2}+\frac{1}{2}(\mu+\nu+2)\left\{\cos\theta-z\sin\theta\left[\frac{1}{4}(\mu+\nu+1)^2-\alpha^2\right]\right\}, \quad (3)$$

which is obtained from (2) by setting $n=0$ and $H_{-1}^{(\mu,\nu)}(z;\alpha,\theta)\equiv 0$. We divide the recursion relation (2) by $\sin\theta\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2-\alpha^2\right]$ and then define the orthonormal version of this polynomial as $\tilde{H}_n^{(\mu,\nu)}(z;\alpha,\theta)=\sqrt{\lambda_n}H_n^{(\mu,\nu)}(z;\alpha,\theta)$ where

$$\frac{\lambda_{n+1}}{\lambda_n}=\frac{(n+1)(n+\mu+\nu+1)(2n+\mu+\nu+3)\left[(2n+\mu+\nu+3)-4\alpha^2\right]}{(n+\mu+1)(n+\nu+1)(2n+\mu+\nu+1)\left[(2n+\mu+\nu+1)-4\alpha^2\right]}, \quad (4)$$

and $\lambda_0=1$. Then $\tilde{H}_n^{(\mu,\nu)}(z;\alpha,\theta)$ satisfies the following symmetric three-term recursion relation

$$z\,\tilde{H}_n^{(\mu,\nu)}(z;\alpha,\theta)=a_n\tilde{H}_n^{(\mu,\nu)}(z;\alpha,\theta)-b_{n-1}\tilde{H}_{n-1}^{(\mu,\nu)}(z;\alpha,\theta)-b_n\tilde{H}_{n+1}^{(\mu,\nu)}(z;\alpha,\theta), \quad (5)$$

where

$$a_n=\left[\cos\theta+\frac{\mu^2-\nu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\right]\Big/\sin\theta\left[\left(n+\tfrac{\mu+\nu+1}{2}\right)^2-\alpha^2\right], \quad (6a)$$

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$$b_n^2=\frac{2^6(n+1)(n+\mu+1)(n+\nu+1)(n+\mu+\nu+1)\big/(\sin\theta)^2\left(2n+\mu+\nu+2\right)^2}{\left(2n+\mu+\nu+1\right)\left(2n+\mu+\nu+3\right)\left[\left(2n+\mu+\nu+1\right)^2-4\alpha^2\right]\left[\left(2n+\mu+\nu+3\right)^2-4\alpha^2\right]}. \tag{6b}$$

The observation that the asymptotics ($n\to\infty$) of these recursion coefficients go like $\mathcal{O}(1/n^2)$ leads to the conclusion that the Jacobi matrix associated with $\tilde{H}_n^{(\mu,\nu)}(z;\alpha,\theta)$ that reads

$$J=\begin{pmatrix} a_0 & b_0 & & & & & \\ b_0 & a_1 & b_1 & & & \mathbf{0} & \\ & b_1 & a_2 & b_2 & & & \\ & & b_2 & a_3 & b_3 & & \\ & & & \times & \times & \times & \\ & \mathbf{0} & & & \times & \times & \times \\ & & & & & \times & \times \end{pmatrix} \tag{7}$$

is a compact operator (in fact, a trace class operator) [15,16]. This implies that the spectrum of J is a countable set $\{z_k, k\in\mathbb{N}\}$ with one accumulation point at zero (i.e., $\lim_{k\to\infty} z_k=0$). The trace class condition implies that $\sum_{k=0}^{\infty}|z_k|$ is finite [15]. Consequently, the orthogonality measure for $\tilde{H}_n^{(\mu,\nu)}(z;\alpha,\theta)$ is a discrete measure supported on this countable set. The asymptotic $\lim_{n\to\infty} z^n$ $\tilde{H}_n^{(\mu,\nu)}(1/z;\alpha,\theta)$ is an entire function with zeros at the points $1/z_k$ [16]. Table 1 shows some of the physical potential functions in quantum mechanics associated with this new polynomial.

Table 1. The physical potential functions associated with the new polynomial $\tilde{H}_n^{(\mu,\nu)}(z;\alpha,\theta)$. The polynomial parameters $\{\mu,\nu,\alpha,\theta\}$ are related to the potential parameters $\{V_0,V_1,V_\pm\}$ as shown, whereas $u_i=2V_i/\eta^2$ and $\varepsilon=2E/\eta^2$.

Title 1	**Title 2**	**Title 3**
entry 1	data	data
entry 2	data	data [1]

If the parameters of the problem that corresponds to the recursion relation (2) requires that $\cos\theta>1$ then we rewrite (2) with $\theta\to i\theta$ and $z\to -iz$ giving

$$\begin{aligned}(\cosh\theta)H_n^{(\mu,\nu)}(z;\alpha,\theta)&=\left\{z\sinh\theta\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2-\alpha^2\right]+\frac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\right\}H_n^{(\mu,\nu)}(z;\alpha,\theta)\\ &+\frac{2(n+\mu)(n+\nu)}{(2n+\mu+\nu)(2n+\mu+\nu+1)}H_{n-1}^{(\mu,\nu)}(z;\alpha,\theta)+\frac{2(n+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+2)}H_{n+1}^{(\mu,\nu)}(z;\alpha,\theta)\end{aligned} \tag{2$'$}$$

Thereafter, we apply the same treatment as we did for (2) above. In Table 1, for example, if $|u_0|\le|u_1|$ then the problem corresponds the recursion (2) otherwise it corresponds to (2)′.

3. The second polynomial

While solving a Heun-type differential equation, we encountered recently another of these new orthogonal polynomials [17]. It is also a four-parameter polynomial, which we designate as $Q_n^{(\mu,\nu)}(z;\alpha,\theta)$. It satisfies the following three-term recursion relation

$$\begin{aligned}(\cos\theta)Q_n^{(\mu,\nu)}(z;\alpha,\theta)&=\left\{z\sin\theta\left[\left(n+\frac{\mu+\nu+1}{2}\right)^2-\alpha^2\right]^{-1}+\frac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\right\}Q_n^{(\mu,\nu)}(z;\alpha,\theta)\\ &+\frac{2(n+\mu)(n+\nu)}{(2n+\mu+\nu)(2n+\mu+\nu+1)}Q_{n-1}^{(\mu,\nu)}(z;\alpha,\theta)+\frac{2(n+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+2)}Q_{n+1}^{(\mu,\nu)}(z;\alpha,\theta)\end{aligned} \tag{8}$$

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where $z\in\mathbb{R}$, $0<\theta\le\pi$ and $n=1,2,...$. Note the inverse power on the square bracket, which constitutes a major difference from the recurrence relation (2). Here too, $Q_0^{(\mu,\nu)}(z;\alpha,\theta)=1$ and $Q_1^{(\mu,\nu)}(z;\alpha,\theta)$ is obtained from (8) by setting $n=0$ and $Q_{-1}^{(\mu,\nu)}(z;\alpha,\theta)\equiv 0$. This polynomial has a purely continuous spectrum over the entire real line. However, it has another version, $G_n^{(\mu,\nu)}(z;\alpha,\beta)$, whose recursion relation is obtained from (8) by the replacement $\theta\to i\theta$ and $z\to -iz$ giving

$$\left(1+\beta^2\right)G_n^{(\mu,\nu)}(z;\alpha,\beta)=\left\{z\left(1-\beta^2\right)\left[\left(n+\tfrac{\mu+\nu+1}{2}\right)^2-\alpha^2\right]^{-1}+\frac{2(\nu^2-\mu^2)\beta}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\right\}G_n^{(\mu,\nu)}(z;\alpha,\beta)$$
$$+\frac{4(n+\mu)(n+\nu)\beta}{(2n+\mu+\nu)(2n+\mu+\nu+1)}G_{n-1}^{(\mu,\nu)}(z;\alpha,\beta)+\frac{4(n+1)(n+\mu+\nu+1)\beta}{(2n+\mu+\nu+1)(2n+\mu+\nu+2)}G_{n+1}^{(\mu,\nu)}(z;\alpha,\beta) \quad (9)$$

where $z\ge 0$ and $\beta=e^{-\theta}$ with $\theta>0$. If α is pure imaginary then the spectrum is purely continuous. However, if α is real then the spectrum is a mix of a continuous positive spectrum and a discrete negative spectrum of finite size *N*, where *N* is the largest integer less than or equal to $|\alpha|-\frac{\mu+\nu+1}{2}$. In this case, the polynomial satisfies a generalized orthogonality relation of the form

$$\int_0^\infty \rho(z)\,G_n^{(\mu,\nu)}(z;\alpha,\beta)\,G_m^{(\mu,\nu)}(z;\alpha,\beta)\,dz+\sum_{k=0}^{N}\omega(k)\,G_n^{(\mu,\nu)}(z_k;\alpha,\beta)\,G_m^{(\mu,\nu)}(z_k;\alpha,\beta)=\lambda_n\delta_{n,m}\,, \quad (10)$$

where $\lambda_n>0$, $\rho(z)$ and $\omega(k)$ are the positive definite continuous and discrete weight functions, respectively. The finite discrete spectrum $\{z_k\}_{k=0}^N$ could be determined from the condition that forces the asymptotics ($n\to\infty$) of $G_n^{(\mu,\nu)}(z;\alpha,\beta)$ to vanish.

Here we can also define the orthonormal version of this polynomial as $\tilde{Q}_n^{(\mu,\nu)}(z;\alpha,\theta)=\sqrt{\lambda_n}\,Q_n^{(\mu,\nu)}(z;\alpha,\theta)$ but now with

$$\frac{\lambda_{n+1}}{\lambda_n}=\frac{(n+1)(n+\mu+\nu+1)(2n+\mu+\nu+3)\left[(2n+\mu+\nu+1)-4\alpha^2\right]}{(n+\mu+1)(n+\nu+1)(2n+\mu+\nu+1)\left[(2n+\mu+\nu+3)-4\alpha^2\right]}. \quad (11)$$

The recursion coefficients of the associated symmetric three-term recursion relation are

$$a_n=\frac{1}{\sin\theta}\left[\cos\theta+\frac{\mu^2-\nu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\right]\left[\left(n+\tfrac{\mu+\nu+1}{2}\right)^2-\alpha^2\right], \quad (12a)$$

$$b_n^2=\frac{(n+1)(n+\mu+1)(n+\nu+1)(n+\mu+\nu+1)\left[(2n+\mu+\nu+1)^2-4\alpha^2\right]\left[(2n+\mu+\nu+3)^2-4\alpha^2\right]}{(2\sin\theta)^2\left(2n+\mu+\nu+1\right)\left(2n+\mu+\nu+2\right)^2\left(2n+\mu+\nu+3\right)} \quad (12b)$$

Note, however, that the associated Jacobi matrix (7) in this case is not compact since the asymptotics of these recursion coefficients go like $a_n\approx n^2$ and $b_n\approx n^2$.

4. Deformation of the Askey scheme of orthogonal polynomials

The polynomial in Section 1 above and the results of our recent studies in [17] and [18], seem to suggest that the type of deformation in the recursion relation like that of the Jacobi polynomial in Eq. (2) is, in fact, common to a larger class of orthogonal polynomials: the Askey scheme of hypergeometric polynomials [13,14]. This scheme consists of two chains of hypergeometric orthogonal polynomials. One of them is a continuous set with the Wilson polynomial at the top of the chain that contains the continuous dual Hahn, continuous Hahn, Meixner-Pollaczek, Jacobi, Laguerre, etc. The other is a discrete set with the Racah polynomial at the top of the chain that includes, the dual Hahn, Hahn, Meixner, Krawtchouk, Charlier, etc. The polynomials in each chain are obtained from that at the top by certain limits of the hypergeometric functions (i.e., ${}_4F_3\to{}_3F_2\to{}_2F_1\to{}_1F_1$). We write the three-term recursion relation of the original polynomials in the scheme generically as follows

$$xP_n^\gamma(x)=a_n^\gamma P_n^\gamma(x)+b_{n-1}^\gamma P_{n-1}^\gamma(x)+c_n^\gamma P_{n+1}^\gamma(x)\,, \quad (13)$$

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where γ stands for a finite set of parameters and x is a continuous or discrete set (finite or countably infinite) or both. The recursion coefficients $\{a_n^\gamma, b_n^\gamma, c_n^\gamma\}$ depend on n and γ but are independent of x. As an example, for the Laguerre polynomial $L_n^\gamma(x)$, x is continuous with $x \geq 0$, $\gamma > -1$ and $a_n^\gamma = 2n+\gamma+1$, $b_n^\gamma = -(n+\gamma+1)$, $c_n^\gamma = -(n+1)$. Now, the deformation of the recursion relation (13) is introduced by modifying it such that it reads

$$x\tilde{P}_n^\gamma(x;\lambda,\alpha) = \left\{a_n^\gamma + \lambda\left[(n+\sigma)^2 - \alpha^2\right]\right\}\tilde{P}_n^\gamma(x;\lambda,\alpha) + b_{n-1}^\mu \tilde{P}_{n-1}^\gamma(x;\lambda,\alpha) + c_n^\mu \tilde{P}_{n+1}^\gamma(x;\lambda,\alpha), \quad (14)$$

where λ is the deformation parameter and σ is a function of the parameter set γ. As an example, the recursion relation (2) above is obtained by deforming that of the Jacobi polynomial $P_n^{(\mu,\nu)}(\cos\theta)$ with $x = \cos\theta$, $\lambda = z\sin\theta$ and $2\sigma = \mu+\nu+1$. Moreover, in Ref. [17] and [18], we also encountered modified versions of orthogonal polynomials in the Askey scheme while searching for series solutions of the following second order linear differential equation

$$x(1-x)(r-x)\left[\frac{d^2y(x)}{dx^2} + \left(\frac{a}{x} - \frac{b}{1-x} - \frac{c}{r-x} + d\right)\frac{dy(x)}{dx}\right] + \left(\frac{A}{x} - \frac{B}{1-x} - \frac{C}{r-x} + xD - E\right)y(x) = 0, \quad (15)$$

where $\{a,b,c,d,r,A,B,C,D,E\}$ are real parameters with $r \neq 0,1$. For $d = 0$, the equation has four regular singular points at $x = \{0,1,r,\infty\}$ and one of its solutions, which we referred to as "*generalized solution*" [17], is written as a series of square integrable basis functions like (1) with the expansion coefficients being modified version of the Wilson polynomial $\tilde{W}_n(z^2;\kappa,\tau,\eta,\xi)$ that satisfies the deformed recursion relation (14) where

$$x = z^2,\ \ \lambda = -r,\ \ 2\sigma = \kappa+\tau+\eta+\xi-1,\ \ \alpha^2 = \tfrac{1}{4}(\kappa+\tau+\eta+\xi-1)^2 - (\kappa+\eta)(\tau+\xi), \quad (16)$$

and the polynomial parameters $\{\kappa,\tau,\eta,\xi\}$ are related to the differential equation parameters in a particular way. In Ref. [19], the Authors refer to $\tilde{W}_n(z^2;\kappa,\tau,\eta,\xi)$ as the "*Racah-Heun polynomial*" but none of its analytic properties was given. On the other hand, for $d \neq 0$ Eq. (15) has four singularities with three regular at $x = \{0,1,r\}$ and one irregular at infinity. In Ref. [18], we obtained a series solution of this differential equation where the expansion coefficients are modified version of the continuous Hahn polynomial $\tilde{p}_n(z;\kappa,\tau,\eta,\xi)$ that satisfies the deformed recursion relation (14) with

$$x = \kappa + \mathrm{i}z,\ \ \lambda = \pm d^{-1},\ \ 2\sigma = \kappa+\tau+\eta+\xi-1,\ \ \alpha^2 = \tfrac{1}{4}(a+b+c-1)^2 - D. \quad (17)$$

The polynomial parameters $\{\kappa,\tau,\eta,\xi\}$ are related to the differential equation parameters $\{a,b,c,d, r,A,B,C,D,E\}$ via one of two alternative ways depending on the $\pm$ sign of λ.

5. Conclusions

Due to the prime significance of these new (or modified) polynomials (along with their discrete versions) to the solution of various problems in physics and mathematics, we urge experts in the field of orthogonal polynomials to study them, derive their analytic properties and write them in closed form (e.g., in terms of the hypergeometric functions). The sought-after properties of these polynomials include the weight function, generating function, asymptotics, orthogonality relation, Rodrigues-type formula, Forward/Backward shift operator relation, zeros, etc.

In Ref. [20], Tcheutia managed to extend the Maple implementation retode of Koepf and Schmersau [21] to cover classical orthogonal polynomials on quadratic or q-quadratic lattices and to treat the polynomial $H_n^{(\mu,\nu)}(z;\alpha,\theta)$ introduced in section 2 above. However, no conclusive results were obtained.

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