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Deformation of the three-term recursion relation and generation of new orthogonal polynomials

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Abstract

We find solutions for a linear deformation of the three-term recursion relation. The orthogonal polynomials of the first and second kind associated with the deformed relation are obtained. The new density (weight) function is written in terms of the original one and the deformation parameters.

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1. Introduction

The use of orthogonal polynomials in the analytic solution of various problems in physics is overwhelming. The reason behind the remarkable presence of these objects may lie in one of the fundamental problems of theoretical physics—the solution of the eigenvalue problem $(H - x)\,|\chi(x)\rangle = 0$, where H is a Hermitian operator and x is real. The solution of this equation for a general observable H of a given physical system is often very difficult to obtain. However, for simple systems or for those with a high degree of symmetry, an analytic solution is feasible. On the other hand, for a large class of problems that model realistic physical systems, the operator H could be written as the sum of two components: $H = H_0 + \tilde{V}$. The 'reference' operator H_0 is often simpler and carries a high degree of symmetry while $\tilde{V}$ is not, but it is usually endowed with either one of two properties. Its contribution is either very small compared to H_0 or is limited to a finite region in configuration or function space. Perturbation techniques are used to provide a numerical evaluation of its contribution in the former case, while algebraic methods are used in the latter [1]. Thus, the analytic problem is confined to finding the solution of the reference H_0-problem

$$(H_0 - x)\,|\psi(x)\rangle = 0. \tag{1}$$

Due to the higher degree of symmetry of this problem, it is frequently possible to find a special basis for the solution space of this equation that supports a tridiagonal matrix representation for H_0. Let $\{\phi_n\}_{n=0}^{\infty}$ be such a basis, which is complete, orthogonal and belongs to the space of square integrable functions. Therefore, we can write the matrix representation of H_0 in this basis as

$$H_0 = \begin{pmatrix} a_0 & b_0 & & & & & \\ b_0 & a_1 & b_1 & & 0 & & \\ & b_1 & a_2 & b_2 & & & \\ & & b_2 & \times & \times & & \\ & & & \times & \times & \times & \\ & 0 & & & \times & \times & \times \\ & & & & & \times & \times \end{pmatrix} \tag{2}$$

where the coefficients $\{a_n, b_n\}_{n=0}^{\infty}$ are real and $b_n \neq 0,\ \forall n$.[1] If we expanded the reference wavefunction as $|\psi(x)\rangle = \sum_n d_n(x)\,|\phi_n\rangle$, then the equivalent matrix representation of the eigenvalue, equation (1), gives the following three-term recursion relation

$$x d_n(x) = a_n d_n(x) + b_{n-1} d_{n-1}(x) + b_n d_{n+1}(x) \qquad n \geqslant 1. \tag{3}$$

This is one way of illustrating the intimate relation between the symmetry of a physical system whose dynamics is described by H_0 in (2), and the theory of orthogonal polynomials associated with this recursion relation. Another approach is found in the studies that investigate the properties of tridiagonal matrices and their relations to quadrature approximation, continued fractions and the theory of orthogonal polynomials [2–6]. In this paper, we want to explore the extent of this relation in the case where the physical system is being subjected to alterations (deformations) of its dynamics. We will show, specifically, that this relation will persist despite a particular kind of one- and three-parameter linear deformation.

Typically, there are two solutions to the recursion relation (3). One results in a regular wavefunction and the other does not. The coefficients of the regular one $d_n(x) \sim p_n(x)$ satisfy a homogeneous initial relation. However, the coefficients of the irregular solution $d_n(x) \sim q_n(x)$ satisfy an inhomogeneous one. These initial relations that complement the above recursion, for $n = 0$, are

$$x p_0 = a_0 p_0 + b_0 p_1 \qquad x q_0 = a_0 q_0 + b_0 q_1 - 1 \tag{4}$$

with $p_0(x) = 1$ and $q_0(x) = 0$. $p_n(x)$ is a polynomial of degree n which is related to the coefficients $d_n(x)$ by $p_n(x) = d_n(x)/d_0(x)$ and is referred to as a 'polynomial of the first kind'. $q_n(x)$, on the other hand, is a polynomial of degree $n-1$ and is referred to as a 'polynomial of the second kind' (see [4], section 2.1, p 8). They also satisfy a Wronskian-like relation (Liouville–Ostrogradskii formula) that reads

$$b_{n-1}[p_{n-1}(x) q_n(x) - p_n(x) q_{n-1}(x)] = 1 \qquad n \geqslant 1.$$

The resolvent operator (Green's function) for this system is formally defined for any complex number z by $G(z) \equiv (H_0 - z)^{-1}$. It has point singularities (respectively, branch cut) on the real line corresponding to the discrete (continuous) spectrum of H_0. Its (0, 0) component can simply be written as the limit of the polynomial ratio

$$G_{00}(z) = -\lim_{n\to\infty}\left[\frac{q_n(z)}{p_n(z)}\right] \tag{5}$$

and has the following continued fraction representation [3–5, 7]

$$G_{00}(z) = -\left\{z - a_0 - {b_0}^2\left[z - a_1 - {b_1}^2\left(z - a_2 - {b_2}^2(\cdots)^{-1}\right)^{-1}\right]^{-1}\right\}^{-1}. \tag{6}$$

[1] These conditions on the coefficients $\{a_n, b_n\}_{n=0}^{\infty}$ will result in a positive definite moment functional associated with the infinite tridiagonal matrix H_0 (Favard's theorem: theorem 4.4 on p 21 of [2]). However, if $b_m = 0$ for some integer $m \geqslant 0$, then H_0 will be the direct sum of a finite $(m+1)\times(m+1)$ matrix and an infinite one resulting in a discrete as well as continuous spectrum.

The density (weight) function $\rho(x)$ associated with these polynomials, which appears in the orthogonality relation $\int_\alpha^\beta \rho(x)p_n(x)p_m(x)\,\mathrm{d}x = \delta_{nm}$, is evaluated using the Stieltjes–Perron inversion formula ([2], p 90, or [5], theorem 2.5, p 11) as the discontinuity of $G_{00}(z)$ across the cut on the real line

$$\begin{aligned}\rho(x) &= \lim_{\varepsilon\to 0}\frac{1}{2\pi\mathrm{i}}[G_{00}(x+\mathrm{i}\varepsilon) - G_{00}(x-\mathrm{i}\varepsilon)]\\ &= \frac{1}{\pi}\,\mathrm{Im}[G_{00}(x+\mathrm{i}0)] \qquad x\in[\alpha,\beta].\end{aligned}\tag{7}$$

Because of the conditions on the coefficients $\{a_n, b_n\}_{n=0}^{\infty}$, it is a positive definite measure according to Favard's theorem ([2], theorem 4.4, p 21). The end points of the interval of orthogonality α and β are determined by the asymptotic behaviour of the recursion coefficients. For one-band density (with 'no gaps'), there is only one pair of asymptotic values for these coefficients (a_∞ and b_∞) from which the two end points are calculated as $a_\infty \pm 2b_\infty$ [8]. However, if the coefficients alternate among k asymptotic values $\left\{a_\infty^i, b_\infty^i\right\}_{i=0}^{k-1}$, then the density will have $k-1$ gaps and the calculation of the end points of the k density bands (the orthogonality intervals) are not so simple [3, 7]. Physically, this corresponds to $k-1$ gaps (forbidden regions) in the continuous energy spectrum of the Hamiltonian H_0. We will illustrate with two examples in section 3, a simple one with a continuous single-band density function and another for a system with two-band density.

2. The deformation

We choose to carry out the development using an alternative notation based on the following set of two-component vector polynomials

$$P_n \equiv \begin{pmatrix} p_n \\ p_{n+1}\end{pmatrix} \qquad Q_n \equiv \begin{pmatrix} q_n \\ q_{n+1}\end{pmatrix}.$$

In this notation, the recursion relation (3) could be rewritten as

$$D_n = \begin{pmatrix} 0 & 1 \\ -\frac{b_{n-1}}{b_n} & \frac{x-a_n}{b_n}\end{pmatrix} D_{n-1} \equiv \Im_n D_{n-1} \qquad n\geqslant 1 \tag{3$'$}$$

where D_n stands for either P_n or Q_n, and $b_n \neq 0$. The initial vectors are

$$P_0 \equiv \begin{pmatrix} 1 \\ \frac{(x-a_0)}{b_0}\end{pmatrix} \qquad \text{and} \qquad Q_0 \equiv \begin{pmatrix} 0 \\ \frac{1}{b_0}\end{pmatrix} \tag{4$'$}$$

Now, we introduce a one-parameter linear deformation of the recursion (3) or, equivalently (3$'$), as the mapping

$$a_0 \to \hat{a}_0 = a_0 + \mu \tag{8}$$

where μ is a real constant parameter. This is equivalent to the transformation

$$(\hat{H}_0)_{nm} = (H_0)_{nm} + \mu\delta_{n_0}\delta_{m_0}. \tag{9}$$

A physical interpretation of this deformation could be given, if H_0 were to represent the dynamics of the given system. For such a system, this deformation could be considered as a model for one-term separable potential coupling [9]. It induces the following change in the orthogonal polynomials so that they form a new complete set of solutions for the deformed recursion relation

$$\hat{P}_n = P_n - \mu Q_n \qquad \hat{Q}_n = Q_n \tag{10}$$

Moreover, using the continued fraction representation of $G_{00}(z)$ in equation (6) we get the following expression for the deformed resolvent: $\hat{G}_{00}(z) = G_{00}(z)/[1 + \mu G_{00}(z)]$, giving the deformed density function as

$$\hat{\rho}(x) = \frac{\rho(x)}{|1 + \mu G_{00}(x + \mathrm{i}0)|^2} \qquad x \in [\alpha, \beta]. \tag{11}$$

The three-parameter deformation, on the other hand, is defined by

$$(\hat{H}_0)_{nm} = (H_0)_{nm} + \mu_+ \delta_{n_0}\delta_{m_0} + \mu_- \delta_{n_1}\delta_{m_1} + \mu_0 \left(\delta_{n_0}\delta_{m_1} + \delta_{n_1}\delta_{m_0}\right) \tag{12}$$

where $\mu_\pm$, μ_0 are real and $\mu_0 \neq -b_0$. It is equivalent to the map

$$a_0 \to \hat{a}_0 = a_0 + \mu_+ \qquad a_1 \to \hat{a}_1 = a_1 + \mu_- \qquad \text{and} \qquad b_0 \to \hat{b}_0 = b_0 + \mu_0 \neq 0 \tag{13}$$

which generates the following polynomial transformations

$$\begin{aligned} \hat{P}_n &= P_n - \frac{b_0}{b_0 + \mu_0}\left[\mu_+ + \frac{\mu_0}{b_0}(x - a_0)\right] Q_n + \frac{\mu_-/b_1}{b_0 + \mu_0}\left[\mu_+ - \frac{\mu_0}{\mu_-}(b_0 + \mu_0) + a_0 - x\right] \tilde{P}_{n-2} \\ \hat{Q}_n &= \frac{b_0}{b_0 + \mu_0} Q_n - \frac{\mu_-/b_1}{b_0 + \mu_0} \tilde{P}_{n-2} \end{aligned} \tag{14}$$

where $\tilde{P}_n = P_n(a_n \to a_{n+2}, b_n \to b_{n+2})$ and $\tilde{P}_{-1} \equiv \binom{0}{1}$, $\tilde{P}_{-2} \equiv \binom{0}{0}$. These polynomials, which are called the 'second associated polynomials' (see [5], section 2.4, p 13) satisfy the recursion relation $\tilde{P}_n = \Im_{n+2}\tilde{P}_{n-1}$, where the 2×2 matrix $\Im_n$ is defined in the recursion relation (3′) above. They are associated with a tridiagonal matrix obtained from H_0 in equation (2) by deleting the first two rows and first two columns (see [4], p 28). They are written in terms of the original polynomials as follows:

$$\tilde{P}_n = -\frac{b_1}{b_0}[P_{n+2} + (a_0 - x)Q_{n+2}] \qquad n \geqslant 0.$$

The deformed resolvent operator can now be written in terms of the original one as

$$\hat{G}_{00}(z) = -\left\{z - a_0 - \mu_+ + (b_0 + \mu_0)^2\left[\mu_- - b_0^2\left(z - a_0 + G_{00}^{-1}(z)\right)^{-1}\right]^{-1}\right\}^{-1} \tag{15}$$

resulting in the deformed density function

$$\hat{\rho}(x) = \left|\left[\frac{1 + (x - a_0)G_{00}(x)}{b_0(b_0 + \mu_0)}\right]\left\{(b_0 + \mu_0)^2 + (x - a_0 - \mu_+)\left[\mu_- - \frac{{b_0}^2 G_{00}(x)}{1 + (x - a_0)G_{00}(x)}\right]\right\}\right|^{-2} \rho(x) \tag{16}$$

where $G_{00}(x) \equiv G_{00}(x + \mathrm{i}0)$ and $x \in [\alpha, \beta]$.

Higher order linear deformation could be pursued following the same formalism presented above for the one- and three-parameter deformations. In each order N, the number of deformation parameters is $N(N + 1)/2$.

3. Examples

As a first example, we consider the simple case where the recursion coefficients are $a_n = 0$, $b_n = 1/2$. These will result in a one-band density whose non-vanishing support is the real interval with end points $a_\infty \pm 2b_\infty = \pm 1$. The three-term recursion relation associated with these coefficients reads $2x d_n(x) = d_{n-1}(x) + d_{n+1}(x)$. The regular solution of

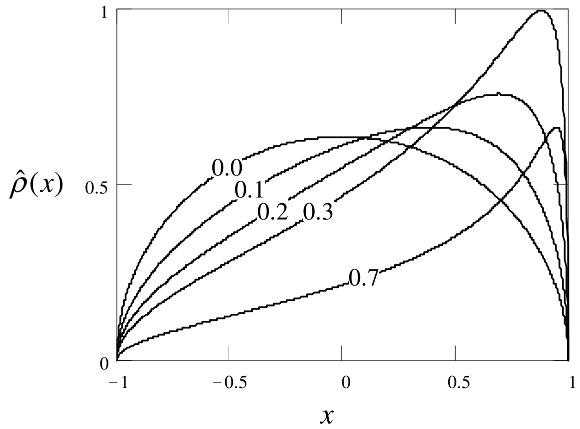

Figure 1. A plot of the one-parameter deformed density of the first example for a range of values of the deformation parameter starting with $\mu = 0$ that corresponds to the undeformed reference density of equation (18).

this recursion is the well-known Chebyshev polynomials [10, 11], which could be written in any one of several alternative forms of which we choose the following

$$p_n(x) = (n+1)\,{}_2F_1\left(-n, n+2; \frac{3}{2}; \frac{1-x}{2}\right) \tag{17}$$

where ${}_2F_1(a, b; c; z)$ is the Gauss hypergeometric function. The irregular solutions (polynomials of the second kind) in this case are simple and could be written as $q_n(x) = 2p_{n-1}(x)$ with $p_{-1}(x) \equiv 0$. The (0, 0) component of the resolvent operator can simply be obtained using the continued fraction representation (6) giving $G_{00}(z) = -2z + 2\sqrt{z^2 - 1}$. Thus, the density function, which is obtained from this $G_{00}(z)$ using relation (7), is

$$\rho(x) = \frac{2}{\pi}\sqrt{1 - x^2} \qquad x \in [-1, +1]. \tag{18}$$

The one-parameter deformation defined in equation (8) or, equivalently, equation (9) produces the following deformed orthogonal polynomials:

$$\hat{p}_n(x) = p_n(x) - 2\mu p_{n-1}(x) \qquad \hat{q}_n(x) = 2p_{n-1}(x). \tag{19}$$

Using equation (11) we obtain the deformed density function

$$\hat{\rho}(x) = \frac{\rho(x)}{1 + 4\mu(\mu - x)} \qquad x \in [-1, +1]. \tag{20}$$

It can easily be shown that the denominator in the above equation is always positive in the orthogonality interval $x \in [-1, +1]$ for all real values of μ. Figure 1 is a plot of this deformed density for a range of values of the deformation parameter starting with $\mu = 0$, which corresponds to the undeformed reference density (18). Negative values of μ produce density plots which are reflections, around the vertical axis $x = 0$, of those with positive values of μ. That is, $\hat{\rho}(x)|_{\mu \to -\mu} = \hat{\rho}(-x)$.

On the other hand, the three-parameter deformation defined by equations (12) or (13) gives the following new orthogonal polynomials:

$$\begin{aligned} \hat{p}_0 &= 1 \qquad \hat{p}_1 = 2\frac{x - \mu_+}{1 + 2\mu_0} \\ \hat{q}_0 &= 0 \qquad \hat{q}_1 = \frac{2}{1 + 2\mu_0} \end{aligned} \tag{21.1}$$

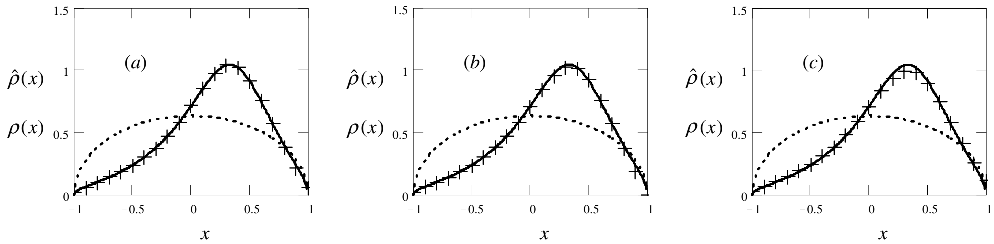

Figure 2. Graphs of the density function $\hat{\rho}(x)$ (solid curve) for the three-parameter deformation of the Chebyshev polynomials superimposed by results from the numerical approximation methods ('+' points). The graphs also show the undeformed reference density function $\rho(x)$ (dotted curve) as given by equation (18). The 'analytic continuation', 'dispersion correction' and 'Stieltjes imaging' methods of [12] were used for the numerical evaluation of the density in figures 2(*a*), (*b*) and (*c*), respectively. The dimension of the deformed matrix $\hat{H}_0$ in the numerical calculations was set to 20. The deformation parameters were assigned the following values: $\mu_+ = 0.2$, $\mu_- = 0.0$, $\mu_0 = -0.1$.

$$\begin{aligned} \hat{p}_n &= p_n - 2\frac{\mu_+ + 2\mu_0 x}{1+2\mu_0} p_{n-1} + \frac{4\mu_-}{1+2\mu_0}\left[-\mu_+ + \frac{\mu_0}{\mu_-}\left(\mu_0 + \frac{1}{2}\right) + x\right](p_n - 2xp_{n-1}) \\ \hat{q}_n &= \frac{2}{1+2\mu_0} p_{n-1} + \frac{4\mu_-}{1+2\mu_0}(p_n - 2xp_{n-1}) \qquad n \geqslant 2 \end{aligned} \tag{21.2}$$

where once again $\mu_0 \neq -1/2$. Note that the combination $p_n - 2xp_{n-1}$ is a polynomial of degree $(n-2)$. The new density function is obtained in terms of the original one using equation (16), which gives

$$\hat{\rho}(x) = \left\{(1+2\mu_0)^2 + 4(\mu_+ - x)\left[x - 2\mu_- + \frac{(\mu_+ - x)}{(1+2\mu_0)^2}\right]\right\}^{-1} \rho(x). \tag{22}$$

The interval of orthogonality is $x \in [-1, +1]$. It is instructive to compare the analytic form of this density function with those that could be obtained independently by any number of possible numerical schemes. In [12], three numerical methods were presented to extract approximate, yet highly accurate, density-of-state information over a continuous range of energies from a finite symmetric Hamiltonian matrix. Starting with a finite version of the deformed matrix $\hat{H}_0$ in equation (12), these methods will be used to evaluate the density function, which will be compared with values obtained from the analytic form, equation (22). The first ('analytic continuation') method relies on the analytic continuation of the finite polynomial ratio approximation, equation (5), of the resolvent operator. The other two ('dispersion correction' and 'Stieltjes imaging') methods are based on the fact that the density function is related to the distribution of the eigenvalues of the finite matrix and one of its submatrices. Figure 2 shows the results of using these three methods with the parameters given in the caption. The agreement with our analytic result is excellent despite the relatively low matrix dimension. Table 1 gives a more precise numerical comparison of the results obtained by the three approximation methods shown graphically in figure 2.

As a second example, we investigate a more interesting case in which the recursion coefficients assume the following real values:

$$a_n = 0 \qquad b_{2n} = \lambda \qquad b_{2n+1} = 1 - \lambda \tag{23}$$

Table 1. This table supplements figure 2 by giving a more precise numerical comparison of the results obtained by the three approximation methods for the deformed density $\hat{\rho}(x)$.

x	$\hat{\rho}(x)$ Exact equation (22)	$\hat{\rho}(x)$ Analytic continuation	$\hat{\rho}(x)$ Dispersion correction	$\hat{\rho}(x)$ Stieltjes imaging
−1.0	0.0000	0.0128	0.0034	0.0109
−0.9	0.0654	0.0657	0.0661	0.0671
−0.8	0.1035	0.1043	0.1042	0.1052
−0.7	0.1429	0.1432	0.1430	0.1447
−0.6	0.1872	0.1874	0.1870	0.1894
−0.5	0.2394	0.2397	0.2389	0.2420
−0.4	0.3023	0.3026	0.3019	0.3052
−0.3	0.3790	0.3790	0.3789	0.3821
−0.2	0.4725	0.4722	0.4730	0.4756
−0.1	0.5852	0.5846	0.5859	0.5872
0.0	0.7153	0.7151	0.7157	0.7148
0.1	0.8531	0.8538	0.8523	0.8479
0.2	0.9746	0.9761	0.9726	0.9635
0.3	1.0426	1.0441	1.0416	1.0276
0.4	1.0236	1.0244	1.0269	1.0108
0.5	0.9151	0.9147	0.9219	0.9094
0.6	0.7490	0.7477	0.7522	0.7506
0.7	0.5665	0.5667	0.5559	0.5724
0.8	0.3938	0.4016	0.3615	0.4007
0.9	0.2347	0.2437	0.1799	0.2416
1.0	0.0000	0.0423	0.0005	0.0503

where $n = 0, 1, 2, \ldots$ and $0 < \lambda \leqslant 1/2$. The $\lambda = 1/2$ case corresponds to the previous example. Using the recursion relation (3) and initial conditions (4), the polynomials of the first and second kind associated with this system are obtained as follows:

$$\begin{aligned}
p_0 &= 1 & q_0 &= 0 \\
p_1 &= \frac{x}{\lambda} & q_1 &= \tfrac{1}{\lambda} \\
p_2 &= \frac{1}{1-\lambda}\left(\frac{x^2}{\lambda} - \lambda\right) & q_2 &= \frac{x}{\lambda(1-\lambda)} \\
p_3 &= \frac{x}{\lambda}\left[\frac{1}{1-\lambda}\left(\frac{x^2}{\lambda} - \lambda\right) - \frac{1-\lambda}{\lambda}\right] & q_3 &= \frac{1}{\lambda^2}\left[\frac{x^2}{1-\lambda} - (1-\lambda)\right]. \\
&\cdots & &\cdots
\end{aligned} \tag{24}$$

It is easy to deduce that $q_n = \lambda^{-1}(p_{n-1})_{\lambda\to 1-\lambda}$. Since the recursion coefficients oscillate asymptotically between the two pairs $(0, \lambda)$ and $(0, 1-\lambda)$, we would expect the density function to consist of two bands. Using equation (6) we obtain the following realization of the resolvent operator:

$$G_{00}(z) = -\frac{1/2}{(1-\lambda)^2}\left[z + \frac{1-2\lambda}{z} - \sqrt{\left(z + \frac{1-2\lambda}{z}\right)^2 - 4(1-\lambda)^2}\,\right]. \tag{25}$$

The four edges of the two density bands are obtained as the zeros of the expression under the square root in the above formula for $G_{00}(z)$. This gives $z = \pm 1$ and $z = \pm(1-2\lambda)$. Indeed,

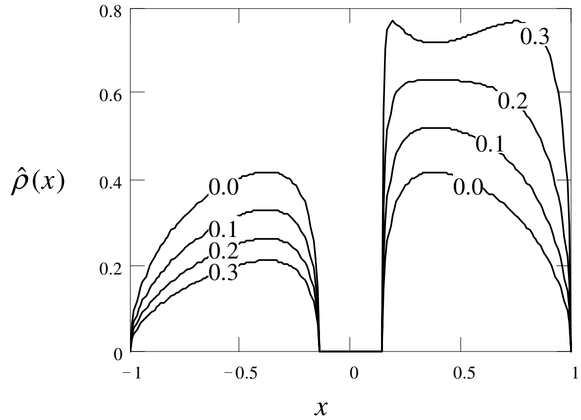

Figure 3. A plot of the one-parameter deformed density of equation (27) with $\lambda = 3/7$ for a range of values of the deformation parameter starting with $\mu = 0$ which corresponds to the two-band reference density of equation (26).

using equation (7), we obtain the two-band reference density as follows:

$$\rho(x) = \begin{cases} -f(x) & -1 \leqslant x < -1 + 2\lambda \\ 0 & -1 + 2\lambda \leqslant x < 1 - 2\lambda \\ +f(x) & 1 - 2\lambda \leqslant x \leqslant +1 \end{cases} \tag{26}$$

where $f(x) = [2\pi x(1-\lambda)^2]^{-1}\sqrt{1-x^2}\sqrt{x^2 - (1-2\lambda)^2}$. Equation (11) gives the following one-parameter deformed density function:

$$\hat{\rho}(x) = \left[1 - \mu\frac{x^2 + 1 - 2\lambda}{x(1-\lambda)^2} + \left(\frac{\mu}{1-\lambda}\right)^2\right]^{-1} \rho(x) \tag{27}$$

where $x \in [-1, -1+2\lambda] \cup [+1-2\lambda, +1]$. For any value of λ in the range $0 < \lambda \leqslant 1/2$, the expression multiplying $\rho(x)$ in the above relation is positive in the two orthogonality intervals for all real values of μ. Figure 3 is a plot of this deformed density for a range of values of the deformation parameter starting with $\mu = 0$ which corresponds to the undeformed reference density, equation (26). Negative values of μ produce plots which are reflections, around the vertical axis $x = 0$, of those with positive values of μ. The deformed polynomials are obtained using equation (10) as follows:

$$\hat{p}_n = p_n - \frac{\mu}{\lambda}(p_{n-1})_{\lambda\to 1-\lambda} \qquad \hat{q}_n = q_n = \lambda^{-1}(p_{n-1})_{\lambda\to 1-\lambda}. \tag{28}$$

The above two examples show how to implement the proposed deformation scheme which starts with a given system of orthogonal polynomials with positive definite measure and generate new orthogonal ones. One-parameter and three-parameter deformations were investigated. A simple system with a continuous one-band density as well as a more involved and interesting one with two-band density were considered.

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