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Explicit representations of Pollaczek polynomials corresponding to an exactly solvable discretization of the hydrogen radial Schrödinger equation

Matias Aunola

Defence Forces Technical Research Centre (PvTT), PO Box 10, FIN-11311, Riihimäki, Finland

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Abstract

We consider an exactly solvable discretization of the radial Schrödinger equation of the hydrogen atom with $l = 0$. We first examine direct solutions of the finite-difference equation and remark that the solutions can be analytically continued into entire functions. A recursive expression for coefficients in the solution is obtained. The next step is to identify the related three-term recursion relation for Pollaczek polynomials. One-to-one correspondence between the spectral and position representations facilitates the evaluation of Pollaczek polynomials corresponding to the discrete spectrum. Finally, we obtain two alternative and explicit expressions for the solutions of the original difference equation.

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1. Introduction

The general solution of the Schrödinger equation, the corresponding energy levels and resulting atomic shell model are taught to all students of quantum mechanics. Experimental and theoretical studies of Rydberg atoms with a single electron have illuminated the wavefunctions and the classical limit of quantum mechanics.

Here, we will concentrate on a specific aspect of theoretical studies, namely discretizations and orthogonal polynomials. Orthogonal polynomials, namely Laguerre polynomials, are already present in the solution of the Schrödinger equation. The subject of orthogonal polynomials related to the hydrogen atom was reviewed in 1991 by Dehesa *et al* in [1]. Apart from polynomials present in the solutions, different kinds of discretizations induce further orthogonal polynomials. The most obvious ones arise from direct discretizations of the Schrödinger equation. Unfortunately, the explicit form of these polynomials is not usually known. The continuum states and L^2 discretizations of the continuum have been studied already in the 1970s [2, 3]. Recently, a corresponding solution for the Dirac–Coulomb problem was presented in [4]. In the context of condensed matter physics discretized Schrödinger equations can also be used as simple models of nanoscale systems [5] or related to the tight-binding approximation [6].

In this paper, we show that the $l = 0$ states of the hydrogen atom can be exactly and explicitly obtained for the symmetric discretization of the second-order derivative. First, this is done by inserting an explicit ansatz in to the difference equation. Later on, we relate the difference equation to the three-term recursion relation for Pollaczek polynomials with specific parameters. Finally, a surprisingly simple and explicit expression is obtained for Pollaczek polynomials and the corresponding solutions of the discretized Schrödinger equation.

2. Initial steps

Let us consider the radial Schrödinger equation for the hydrogen atom, i.e.,

$$-\frac{\hbar^2 R''(r)}{2m} - \frac{\hbar^2 R'(r)}{mr} - \frac{e^2 R(r)}{4\pi\varepsilon_0 r} + \frac{\hbar^2 l(l+1)R(r)}{2mr^2} = ER(r). \tag{1}$$

In so-called natural units and for $l = 0$ the equation simplifies to

$$-\frac{u''(r)}{2} - \frac{u(r)}{r} = Eu(r), \tag{2}$$

where $u(r) = rR(r)$. The simple eigenvalues and well-known solutions are expressible in terms of associated Laguerre polynomials of the first kind

$$u_n(r) = rL_n^1(2r/n)\,e^{-r/n} = e^{-r/n}\sum_{k=1}^{n}\frac{(-2/n)^{k-1}}{k!}\binom{n-1}{k-1}r^k, \qquad E_n = -\frac{1}{2n^2}, \tag{3}$$

where $n = 1, 2, \ldots$. Next, we discretize this equation using the symmetric second-order difference and obtain a finite-difference equation

$$-\frac{u(r-\delta) - 2u(r) + u(r+\delta)}{2\delta^2} - \frac{u(r)}{r} = E(\delta)u(r). \tag{4}$$

In the following section, we lift the restrictions that r and δ must lie on the positive axis and allow complex values for both. Of course, any solution of equation (4) multiplied by an arbitrary function with period δ is still a solution. Nevertheless, we will concentrate on solutions and eigenvalues that tend to corresponding classical solutions in the limit $\delta \to 0$.

3. Solutions in coordinate representation

For nonzero values of δ we note that functions $u(r)$ are also solutions of

$$u(r-\delta)/2 + u(r+\delta)/2 + \delta^2 u(r)/r = \mu u(r), \tag{5}$$

where $\mu = -\delta^2 E + 1$. This problem has been studied by Berezin in the case of purely imaginary δ in [7]. We discovered the existence of an explicit solution in [8]. Here, a more transparent and instructive derivation is given and we are able to obtain a new, recursive formula for arbitrary terms in the solution.

Let us insert an ansatz

$$u(r) = e^{\beta r}\sum_{k=1}^{n}\alpha_k r^k, \tag{6}$$

into equation (5) and assume $\alpha_k \neq 0$, which obviously corresponds to the solution $u_n(r)$ in equation (3). Now the equations must hold identically in r so each coefficient of r^j must vanish. This yields

$$\sum_{k=\max(1,j-1)}^{n} \gamma_{j,k}\alpha_k = 0, \qquad \gamma_{j+1,k} := \delta^{k-j}\binom{k}{j}(\mathrm{e}^{\beta\delta} + (-1)^{k-j}\,\mathrm{e}^{-\beta\delta})/2 - \mu\gamma_{k,j} + \delta^2\gamma_{k,j+1} \tag{7}$$

for $j = 1, \ldots, n+1$. The $(n+1)$th equation requires that $\alpha_n[\cosh(\delta\beta) - \mu] = 0$, so we find $\mu = \cosh(\delta\beta)$. Next equation is then simplified to $\alpha_n[n\delta^{-1}\sinh(\delta\beta) + 1] = 0$. These equations now yield

$$\mu_n(\delta) = \sqrt{1 + (\delta/n)^2}, \qquad \beta_n(\delta) = -\mathrm{arsinh}(\delta/n)/\delta \tag{8}$$

in agreement with [8]. The classical limits $E_n(\delta) \to -1/2n^2$ and $\beta_n(\delta) \to -1/n$ are also satisfied. The remaining $n-1$ equations can be used in order to solve the constants α_k with $k = 1, \ldots, n-1$. Note that the present derivation is both simpler and more exhaustive than the previous one, which was based on an intelligent guess concerning the identity of terms in the power series used. All eigenvalues and constants in the exponential part are identical to those given in equation (8).

The general solution to equation (5) now becomes

$$u_n^{(\delta)}(r) = \left(\sum_{k=1}^{n} \ell_k^{(n)}\alpha_k^{(n,\delta)} r^k\right)\exp(-r\,\mathrm{arsinh}(\delta/n)/\delta), \qquad \ell_k^{(n)} := \frac{(-2/n)^{k-1}}{k!}\binom{n-1}{k-1}. \tag{9}$$

The coefficients $\{\alpha_k^{(n,\delta)}\}$ are of the form

$$\alpha_{n-k}^{(n,\delta)} = (1 + \delta^2/n^2)^{(k-2k')/2}\sum_{m=0}^{k'} \alpha_{n-k,m}^{(n)}\delta^{2m}, \tag{10}$$

where $\alpha_{k,0}^{(n)} = 1$ and $k' = \lfloor k/2 \rfloor$, i.e., $k/2$ if k is even and $(k-1)/2$ if k is odd. In addition, we find

$$\alpha_{n-k,m}^{(n)} = n^{-2m}\binom{\lfloor k/2 \rfloor}{m}\frac{P(2m-1)(n-k)!}{(n-k+2m-1)!}, \tag{11}$$

where $P(2m-1)$ is a polynomial of order $2m-1$ such that the coefficient of x^{2m-1} is equal to unity. The general form of the leading terms is given by

$$\alpha_n^{(n,\delta)} = 1 \tag{12}$$

$$\alpha_{n-1}^{(n,\delta)} = \sqrt{1 + \delta^2/n^2} \tag{13}$$

$$\alpha_{n-2}^{(n,\delta)} = 1 + \frac{(3n-1)\delta^2}{3n^2(n-1)} \tag{14}$$

$$\alpha_{n-3}^{(n,\delta)} = \sqrt{1 + \delta^2/n^2}\left(1 + \frac{n\delta^2}{n^2(n-2)}\right) \tag{15}$$

$$\alpha_{n-4}^{(n,\delta)} = 1 + \frac{2(n-1)\delta^2}{n^2(n-3)} + \frac{(15n^3 - 30n^2 + 5n + 2)\delta^4}{15n^4(n-1)(n-2)(n-3)}. \tag{16}$$

Here n is an arbitrary state index, so once $\alpha_{n-k}^{(n,\delta)}$ has been obtained, we have exact expressions for $k+1$ leading polynomial terms in any eigenfunction. We have now obtained explicit expressions for $\alpha_{n-k}^{(n,\delta)}$ when $k \leqslant 125$ and $\alpha_{k,m}^{(n)}$ for $m \leqslant 23$ with arbitrary k. In order to do this the underlying symmetries of the coefficients have to be exploited efficiently. Some of this work was already done in [8], and one can find explicit values of terms up to $k \leqslant 49$ and $m \leqslant 10$ in the addendum.

We proceed by noting that the innermost coefficients, $\{\alpha^{(n)}_{n-k,m}\}$, yield a general solution to the present difference equation. We define

$$C_{n,k,l} := \frac{(-n/2)^k n!}{k!l!(n-k-l)!}\prod_{m=1}^{k}(n-m), \tag{17}$$

and assume that all coefficients up to level $\alpha^{(n)}_{n-(k-1),m}$ are known. The requirement that the coefficient for each power of δ cancels separately and some algebra yields explicit expressions for the coefficients on the next level. For even values of k we find

$$\alpha^{(n)}_{n-k,m\geqslant 1} = \left(-\sum_{l=k'-m}^{k'-1} C_{n,2l,k+1-2l}\alpha^{(n)}_{n-2l,l+m-k'}\Big/n + \sum_{l=k'-m-1}^{k'-1} C_{n,2l+1,k-2l}\alpha^{(n)}_{n-2l-1,l+m-k'+1}\right.$$
$$\left. + \sum_{l=k'-m}^{k'-1} C_{n,2l+1,k-2l}\alpha^{(n)}_{n-2l-1,l+m-k'}\Big/n^2\right)\Bigg/ (C_{n,k,1}/n - C_{n,k,0}). \tag{18}$$

Correspondingly for odd values of k this yields

$$\alpha^{(n)}_{n-k,m\geqslant 1} = \left(-\sum_{l=k'-m}^{k'-1} C_{n,2l+1,k-2l}\alpha^{(n)}_{n-2l-1,l+m-k'}\Big/n\right.$$
$$\left. + \sum_{l=k'-m}^{k'} C_{n,2l,k+1-2l}\alpha^{(n)}_{n-2l,l+m-k'}\right)\Bigg/ (C_{n,k,1}/n - C_{n,k,0}). \tag{19}$$

Here, $\alpha^{(n)}_{k,0} = 1$ and impossible coefficients are taken to be zero. The recursive equations do yield the general solution, but the complexity of equations grows at an exponential rate. Thus, it has been necessary to use even higher order symmetries to reduce the number of equations and reach the present order $k = 125$. All calculations have been performed using the symbolic mathematical software MATHEMATICA.

By restricting the allowed values of r to the set $\{k\delta\}_{k=1}^{\infty}$, we transform the problem into an eigenvalue problem for an infinite tridiagonal matrix. By denoting $u^n_k := u^{(\delta)}_n(k\delta)$, we see that the vector $\{u^n_k\}_{k=1}^{\infty}$ is an eigenvector of the matrix

$$H_{kk} = \delta/k, \qquad H_{k,k+1} = H_{k+1,k} = 1/2, \qquad k = 1, 2, \ldots \tag{20}$$

corresponding to the eigenvalue $\mu_n = \sqrt{1 + (\delta/n)^2}$. In addition, the exponential part of the solution simplifies to

$$\exp(-k\delta \operatorname{arsinh}(\delta/n)/\delta) = \left(\sqrt{1 + (\delta/n)^2} - \delta/n\right)^k. \tag{21}$$

Results from numerical diagonalization agree with our results within numerical precision, as long as convergence can be reached. For δ real and positive, normalized eigenvectors form an orthonormal basis of ℓ^2.

The polynomial part of the eigenvectors define a discretized version of the corresponding associated Laguerre polynomials L^1_n. It is not clear whether a three-term recursion relation exists for these polynomials.

4. Solutions in spectral representation

The polynomial character of the exponential part shown in equation (21) contains both the eigenvalue μ and the discretization parameter, which indicates that we should also examine the problem with respect to the spectral variable. It turns out that the problem at hand corresponds to a special case of the Pollaczek polynomials [9]. They satisfy the three-term recursion relation

$$(j+1)P_{j+1}^{\lambda}(x;a,b) = 2[(j+\lambda+a)x+b]P_j^{\lambda}(x;a,b) - (j+2\lambda-1)P_{j-1}^{\lambda}(x;a,b), \tag{22}$$

where $j > 0$, and initial conditions

$$P_0^{\lambda}(x;a,b) = 1, \qquad P_1^{\lambda}(x;a,b) = 2(\lambda+a)x+b. \tag{23}$$

From equation (20) we obtain the recursion relation

$$(j+1)u_{j+1} = 2[(j+1)x-\delta]u_j - (j+1)u_{j-1}, \qquad j(=k-1) > 0, \tag{24}$$

and identify the parameters $\lambda = 1$, $a = 0$ and $b = -\delta$. The discrete spectrum agrees with the calculations performed above, i.e.,

$$x_m = \sqrt{1+\delta^2/(m+1)^2}, \qquad m = 0, 1, \ldots. \tag{25}$$

We have not yet studied the absolutely continuous spectrum in the range $[-1, 1]$.

The explicit formula for Pollaczek polynomials reads

$$P_n^{\lambda}(\cos\theta;a,b) = \sum_{k=0}^{n} \frac{(-\lambda+\mathrm{i}\Phi(\theta))_k(\lambda+\mathrm{i}\Phi(\theta))_{n-k}}{k!(n-k)!}\,\mathrm{e}^{\mathrm{i}\theta(2k-n)}, \tag{26}$$

where $x := \cos\theta$, $\Phi(\theta) = (a\cos\theta+b)/\sin\theta$ and $(A)_k = A(A+1)\cdots(A+k-1)$. The orthogonality of Pollaczek polynomial is defined with respect to the interval $[-1, 1]$, where $\cos\theta$ and $\sin\theta$ are easily defined. Here, it would be tempting to use

$$\sin\theta = \pm\mathrm{i}\delta/(m+1), \tag{27}$$

which yields simple terms to be inserted in equation (26). Nevertheless, the correct way to do this as well as the corresponding interpretation are not obvious to us.

Below, we obtain a simpler way to express the polynomials $P_j(x) := P_j^1(x;0,-\delta)$ for $x\,(>1)$ within the discrete spectrum (25). The results of the previous section show that we can write

$$P_j(x_m) = (x_m - \delta/(m+1))^{j-m} Q_j^m(x_m), \tag{28}$$

where Q_j^m is a polynomial of degree m. By extracting the polynomials Q_j, we can reconstruct the corresponding Pollaczek polynomials. The next step is to evaluate polynomial relations with respect to the index j, i.e., express the coefficients of the polynomials in as functions of j. Thus, we write

$$P_j(x_m) = (j+1)\sum_{l=0}^{j}\binom{j}{l}(x_m)^{j-l}\left(-\frac{\delta}{m+1}\right)^l \beta_{m,l} \tag{29}$$

$$Q_j(x_m) = (j+1)\sum_{l=0}^{m}\binom{m}{l}(x_m)^{m-l}\left(-\frac{\delta}{m+1}\right)^l \gamma_{j,l}. \tag{30}$$

Both factors $\beta_{j,l}$ and $\gamma_{m,l}$ appear to be quite complicated at first. Some general features can be gleaned out, but the breakthrough is achieved in three steps. First is the observation that $\gamma_{j,l} = \beta_{j,l}$ and the next amounts to the symmetry $\beta_{j,l} = \beta_{l,j}$. Finally, we find

$$\beta_{j,m} = \sum_{l=0}^{\min(j,m)} \frac{2^l}{l+1}\binom{j}{l}\binom{m}{l}. \tag{31}$$

This is the solution we have been looking for, explicitly,

$$P_j(x_m) = (j+1)\sum_{l=0}^{j}(x_m)^{j-l}\left(\frac{-\delta}{m+1}\right)^l\left[\binom{j}{l}\sum_{k=0}^{\min(m,l)}\frac{2^k}{k+1}\binom{m}{k}\binom{l}{k}\right]$$

$$= (j+1)\left(x_m-\frac{\delta}{m+1}\right)^{j-m}\sum_{l=0}^{m}(x_m)^{m-l}\left(\frac{-\delta}{m+1}\right)^l \times\left[\binom{m}{l}\sum_{k=0}^{\min(j,l)}\frac{2^k}{k+1}\binom{j}{k}\binom{l}{k}\right]. \tag{32}$$

The first expression is more convenient for $j \leqslant m$, while the second is more compact for $j > m$. Note that expressions are manifestly identical for $j = m$. The unnormalized, general solution to the matrix eigenvalue problem (20) now simplifies to

$$u_k^n = P_{k-1}(x_{n-1}), \qquad \mu_n = x_{n-1}. \tag{33}$$

For real values of δ the solutions satisfy the orthogonality relation

$$\sum_{k=1}^{\infty} u_k^n u_k^{n'} \propto \delta_{n,n'} \tag{34}$$

and normalization requires that

$$\sum_{k=1}^{\infty} \left|u_k^n\right|^2 = 1. \tag{35}$$

For small values of j or m we can be sure that Pollaczek polynomial does satisfy the recursion relation. The solutions for spectral and coordinate representations are identical because they are solutions to the same difference equation. Thus, in the limit $\delta \to 0$, the Pollaczek polynomials tend to Laguerre polynomials with corresponding exponential parts, even if the variables x and r do not coincide. The extraction process guarantees that each term has been uniquely and correctly identified with corresponding powers of x_m and $-\delta/(m+1)$. Next, we identified several sets of equations that these coefficients satisfy. This allowed us to construct further coefficients in the series without redoing the extraction process. As the final step, the explicit expressions were conjectured and verified against known results. The general solution to equation (5) can be considered as a partially proven conjecture.[1]

5. Discussion

We have examined a simple discretization of the radial Schrödinger equation and shown that it is exactly solvable. We were able to obtain an explicit solution both in terms of the radial coordinate as well as the spectral variable, i.e., the eigenvalue. In future, one can simply use the existing solution, e.g., in the form of a piece of computer code based on equation (32). Simultaneously, we derived simple expressions to Pollaczek polynomials $P_j^1(x; 0, -\delta)$ for the discrete mass points x_m. Initial steps of the present approach are due to earlier research on the discretized 1D harmonic oscillator, where we obtained asymptotical representations of Mathieu functions [10]. Much work still remains and alternative approaches should be applied to these problems.

As a final note, we state that the present discretization of the Schrödinger equation can also be used when visualizing hydrogen radial wavefunctions. The possibility of comparing a

[1] The required intermediate steps are available at request from Matias.Aunola@pvtt.mil.fi.

numerical algorithm against exact results is not too common, especially if exact results are for the algorithm itself. Of course, it is not possible to carry the recursion either to infinite order or with infinite precision.

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