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Discrete Quantum Harmonic Oscillator

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Abstract: In this paper, we propose a discrete model for the quantum harmonic oscillator. The eigenfunctions and eigenvalues for the corresponding Schrödinger equation are obtained through the factorization method. It is shown that this problem is also connected with the equation for Meixner polynomials.

Keywords: difference equations; discrete Schrödinger equation; quantum harmonic oscillator; classical discrete orthogonal polynomials; factorization method; Meixner polynomials

1. Introduction

The aim of this paper is to propose a discrete version of the stationary Schrödinger equation for the quantum harmonic oscillator and to solve the associated spectral problem, i.e., to find the eigenfunctions and eigenvalues for the corresponding Hamiltonian. There are in the literature several ways for introducing such a discretization (see, for example, [1–3]). The most obvious one consists of simply substituting in place of the quadratic potential $V(x) = x^2$ of the continuous case the function $V(n) = n^2$ in the standard central difference expression for the corresponding Hamiltonian. In general, it is not simple to find explicit expressions for the corresponding eigenfunctions and eigenvalues. Moreover, even if we would find them, it is not always true that the spectrum in the discrete case will satisfy the fundamental property of the continuous case, namely that the associated energy levels form a discrete set of equidistant eigenvalues. The discrete version of the infinite square well and the relationship with the tight-binding model was studied by Boykin and Klimeck [4]. In [5], some properties of the mapping of the discrete Schrödinger equation into a two-term wave evolution equation have been considered. In [6,7], the authors showed that supersymmetric quantum mechanics is a simple, powerful tool for generating potentials with known spectra starting from a given initial solvable one. In [8], the factorization method has been used to deal with second-order difference equation on time scales. The construction of creation and annihilation operators for the harmonic oscillator and hydrogen atom on the lattice starting from Rodrigues formula was done by Lorente [2]. The exact discretization of the Schrödinger equation was proposed in [9] based on Fourier transforms.

In a recent paper, we introduced a discrete version of Darboux transformations and Crum formula for generating new potentials starting from an initial solvable one [10], and included a different proposal for the discrete harmonic oscillator potential given by $V(n) = n^2 + n + 1$, which has an explicit solution for zero energy. Motivated by this, here we use such an alternative choice of discretization and we solve the corresponding discrete stationary Schrödinger equation. We show that the associated spectrum consists of an infinite set of equidistant energy levels, as it happens in the continuous case.

To do that, we employ the factorization method for generating a sequence of Hamiltonians whose eigenfunctions are interrelated through first-order difference operators. We also show that the solution to the eigenvalue problem is connected with the difference equation for the Meixner polynomials.

2. Preliminaries

In this section, we recall some notation from difference calculus and difference equations, and well-known facts about classical discrete orthogonal polynomials.

We denote by $\ell(\mathbb{Z};\mathbb{R})$ and $\ell(\mathbb{Z};\mathbb{C})$ the sets of real- and complex-valued sequences, respectively. We use the standard notation for shift operators as well as forward and backward difference operators acting on $\ell(\mathbb{Z};\mathbb{R})$ and $\ell(\mathbb{Z};\mathbb{C})$ by

$$\begin{aligned} &T^{\pm}\psi(n) := \psi(n \pm 1),\\ &\Delta\psi(n) := \left(T^{+} - \mathbb{I}\right)\psi(n) = \psi(n+1) - \psi(n),\\ &\nabla\psi(n) := \left(\mathbb{I} - T^{-}\right)\psi(n) = \psi(n) - \psi(n-1). \end{aligned}$$

Thus, the forward second difference is given by

$$\Delta^2\psi(n) = \psi(n+2) - 2\psi(n+1) + \psi(n).$$

A linear second-order difference equation can be written in general as follows

$$a(n)\psi(n+2) + b(n)\psi(n+1) + c(n)\psi(n) = 0,$$

where $\{a\}$, $\{b\}$ and $\{c\}$ are given sequences. It is well-known how to solve the above equation when the coefficients are constant (see, e.g., [11]).

We want to propose here a discrete version of the Schrödinger equation for the harmonic oscillator

$$\left(-\frac{d^2}{dx^2} + x^2\right)\psi(x) = \lambda\psi(x).$$

There are different approaches for discretizing the one-dimensional time-independent Schrödinger equation (see [4,5,9]). Very often, a discretization appears from the standard central difference formula

$$\left(-\Delta\nabla + n^2\right)\psi(n) = \lambda\psi(n).$$

In our considerations below, we modify the above equation as follows

$$\left(-\Delta^2 + (n^2 + n + 1)\right)\psi(n) = \lambda\psi(n+1),$$

which can be written explicitly as

$$-\psi(n+1) + (2-\lambda)\psi(n) + n(n-1)\psi(n-1) = 0, \tag{1}$$

i.e., we consider one step forward shifted eigenfunctions.

In addition, there is a relationship of Equation (1) with classical orthogonal polynomials of a discrete variable. Indeed, it is well-known that the equation of hypergeometric type

$$\sigma(n)\Delta\nabla\psi_m(n) + \tau(n)\Delta\psi_m(n) + \lambda_m\psi_m(n) = 0, \tag{2}$$

describes such discrete classical orthogonal polynomials as Charlier, Meixner, Kravchuk, and Hahn polynomials, among others (see [12,13]). The sequences $\sigma(n)$ and $\tau(n)$ are second- and first-degree polynomials, respectively, and

$$\lambda_m = -m\left(\tau' + \frac{m-1}{2}\sigma''\right).$$

If $\sigma(n)\rho(n)n^i\big|_{n=a,b} = 0$, for all $i \in \mathbb{N} \cup \{0\}$, and the function ρ satisfies the analogue of Pearson equation

$$\Delta\left(\sigma(n)\rho(n)\right) = \tau(n)\rho(n),$$

then the polynomial solutions of Equation (2) are orthogonal with respect to the weight function ρ

$$\left\langle \psi^m | \varphi^l \right\rangle = \sum_{n=a}^{b-1} \psi^m(n)\varphi^l(n)\rho(n) = \delta_{ml} d_m^2.$$

In particular, the Meixner polynomials are important in our research [14,15]. The Meixner polynomials $M_m^{\gamma,\mu}(n)$ are obtained from the following sequences

$$\sigma(n) = n, \tag{3}$$
$$\tau(n) = (\mu - 1)n + \mu\gamma, \tag{4}$$

and constants

$$\lambda_m = (1 - \mu)m. \tag{5}$$

In this case, the scalar product is defined on the interval $[a, b] = [0, \infty)$. These polynomials can be also defined through a generating function in the way

$$\left(1 - \frac{t}{\mu}\right)^n (1 - t)^{-n-\gamma} = \sum_{m=0}^{\infty} \frac{1}{m!} M_m^{\gamma,\mu}(n) t^m.$$

The explicit formulas for the Meixner polynomials are the following

$$M_m^{\gamma,\mu}(n) = (-1)^m m! \sum_{k=0}^{m} \binom{n}{k} \binom{-n-\gamma}{m-k} \mu^{-k}.$$

They can be also expressed in terms of the hypergeometric series

$${}_mF_n\left(\begin{array}{cccc} a_1, & \ldots, & a_m, \\ b_1, & \ldots, & b_n \end{array} \middle| x\right) := \sum_{k=0}^{\infty} = \frac{(a_1)_k \ldots (a_m)_k}{(b_1)_k \ldots (b_n)_k} \frac{x^k}{k!}, \quad m, n \in \mathbb{N},$$

by

$$M_m^{\gamma,\mu}(n) = (\gamma)_m {}_2F_1\left(\begin{array}{c} -m, -n \\ \gamma \end{array} \middle| 1 - \frac{1}{\mu}\right) =$$

$$= (\gamma)_m \sum_{k=0}^{\infty} \frac{1}{k!} \frac{(-m)_k(-n)_k}{(\gamma)_k} \left(1 - \frac{1}{\mu}\right)^k,$$

where the Pochhammer symbol is defined by

$$(a)_k = a(a+1)\ldots(a+k-1) \quad \text{for} \quad k > 0$$

and $(a)_0 = 1$.

3. Sequence of Discrete Quantum Harmonic Oscillators

Let $\ell_k(\mathbb{Z}; \mathbb{C})$, $k \in \mathbb{Z}$, be the sets of complex-valued sequences $\{\psi_k\}$ defined on $\mathbb{Z}$ and square-summable $\langle \psi_k | \psi_k \rangle_k < +\infty$, with the scalar products

$$\langle \psi_k | \varphi_k \rangle_k := \sum_{n=a}^{b-1} \overline{\psi_k(n)} \varphi_k(n) \rho_k(n), \tag{6}$$

where ρ_k are weight functions.

The main object of our considerations is the sequence of second-order operators $\mathbf{H_k} : \ell_k(\mathbb{Z}, \mathbb{C}) \longrightarrow \ell_k(\mathbb{Z}, \mathbb{C})$ given by

$$\mathbf{H_k} = -T^+ + n(n-1-k)T^- + 2 - k$$

and the problem of eigenvalues for these operators

$$\mathbf{H_k}\psi_k^m(n) = \lambda_k^m \psi_k^m(n). \tag{7}$$

Here, m labels the energy levels and associated eigenfunctions. In this sequence, we recognize the problem of eigenvalues for the discrete quantum harmonic oscillator (Equation (1)) for $k = 0$.

The family of operators $\mathbf{H_k}$ can be factorized as a product of first-order operators

$$\mathbf{H_k} = \mathbf{A_k^*}\mathbf{A_k} + \alpha_k = \mathbf{A_{k+1}}\mathbf{A_{k+1}^*} + \alpha_{k+1},$$

where the annihilation and creation operators $\mathbf{A_k} : \ell_k(\mathbb{Z}, \mathbb{C}) \longrightarrow \ell_{k-1}(\mathbb{Z}, \mathbb{C})$ and $\mathbf{A_k^*} : \ell_{k-1}(\mathbb{Z}, \mathbb{C}) \longrightarrow \ell_k(\mathbb{Z}, \mathbb{C})$ are given by

$$\begin{aligned} \mathbf{A_k} &= T^+ + (n-k)\mathbb{I}, \\ \mathbf{A_k^*} &= nT^- - \mathbb{I}. \end{aligned}$$

In turn, the constants α_k are given by

$$\alpha_k = 2 - 2k.$$

This type of factorizations was presented in detail for the general situation in a discrete case in [16–18] and in [19–21] for the τ- and q-cases too. It is based on classical methods taken from the work of some founders of quantum mechanics such as Schrödinger [22] (see also [23–25]).

In general, the creation operator $\mathbf{A_k^*}$ is the adjoint of the annihilation operator $\mathbf{A_k}$ relative to the scalar product (6), where the weight functions ρ_k satisfy the Pearson type equations (see [17]). In our case, we have

$$\Delta\left(n\rho_k(n)\right) = \left(-\frac{1}{n-k} - n\right)\rho_k(n), \tag{8}$$

and the recursion relation

$$\rho_{k-1}(n) = -\frac{1}{n-k}\rho_k(n). \tag{9}$$

The boundary conditions read as follows

$$a\rho_k(a) = b\rho_k(b) = 0.$$

If ρ_k were a positive weight function, then the operator $\mathbf{H_k}$ would be self-adjoint and its eigenfunctions corresponding to different eigenvalues would be orthogonal

$$\left\langle \psi_k^m | \psi_k^l \right\rangle_k = 0 \quad \text{for} \quad m \neq l.$$

From above expression, after a direct calculation, we find

$$\rho_k(n) = \begin{cases} \dfrac{(-1)^{n+k}}{n!(n-k-1)!} & \text{for} \quad n > k \\ 0 & \text{for} \quad n \leq k \end{cases}, \tag{10}$$

$$a = k, \tag{11}$$

$$b = \infty. \tag{12}$$

We see that the function ρ_k is not positive, i.e., $\langle\cdot|\cdot\rangle_k$ is not a scalar product, but it can be interpreted as a pseudo-scalar product. In this case, an explicit calculation using Equations (8) and (9) also yields

$$\langle\psi_{k-1}|\mathbf{A_k}\varphi_k\rangle_{k-1} = \sum_{n=k}^{\infty}\overline{\psi_{k-1}(n)}\rho_{k-1}(n)\left(T^{+}+n-k\right)\varphi_k(n) = \tag{13}$$

$$= \sum_{n=k}^{\infty}\overline{\psi_{k-1}(n)}\varphi_k(n+1)\rho_{k-1}(n) + \sum_{n=k}^{\infty}\overline{\psi_{k-1}(n)}\left(n-k\right)\varphi_k(n)\rho_{k-1}(n) =$$

$$= \sum_{n=k+1}^{\infty} n\overline{\psi_{k-1}(n-1)}\varphi_k(n)\rho_k(n) - \sum_{n=k+1}^{\infty}\overline{\psi_{k-1}(n)}\varphi_k(n)\rho_k(n) =$$

$$= \sum_{n=k+1}^{\infty}\varphi_k(n)\rho_k(n)\left(nT^{-}-1\right)\overline{\psi_{k-1}(n)} = \langle\mathbf{A^*_k}\psi_{k-1}|\varphi_k\rangle_k\,.$$

Let us note that there exists an important class of solutions of Equation (7) such that $\lambda_k^0 = \alpha_k$. If we consider the first-order difference equation

$$\mathbf{A_k}\psi_k^0(n) = 0, \tag{14}$$

then any nonzero solution to this equation is automatically a solution of Equation (7) with eigenvalue $\lambda_k^0 = \alpha_k$. It is easy to find now a solution to Equation (14) (the so-called ground state)

$$\psi_k^0(n) = (-1)^n(n-k-1)!C_k \quad \text{for} \quad n > k, \tag{15}$$

where C_k is a constant. If $k \geq 0$, then the series $\langle\psi_k^0|\psi_k^0\rangle_k$ is convergent. The operators $T^{\pm}$ operate on the level of ground states for different k as follows:

$$\ldots\psi_k^0 \underset{-T^{+}}{\overset{-T^{-}}{\rightleftarrows}} \psi_{k+1}^0 \underset{-T^{+}}{\overset{-T^{-}}{\rightleftarrows}} \psi_{k+2}^0\cdots$$

Moreover, the function $\psi_k^0(n)$ can be used to construct the *excited state* solutions of Equation (7) through the formula

$$(-1)^m\psi_{k+m}^m(n) = \mathbf{A^*_{k+m}}\ldots\mathbf{A^*_{k+2}}\mathbf{A^*_{k+1}}\psi_k^0(n) = \left(nT^{-}-\mathbb{I}\right)^m\psi_k^0(n)$$

or, equivalently, $\psi_k^m(n) = (nT^{-}-\mathbb{I})^m\,\psi_k^0(n+m)$. These eigenfunctions correspond to the eigenvalues $\lambda_k^m = \alpha_{k-m} = 2-2k+2m$. For example, a straightforward calculation leads to

$$\begin{aligned}
&\psi_k^1(n) = (2n-k)\psi_k^0(n) \quad \text{for} \quad \lambda_k^1 = -2k+4,\\
&\psi_k^2(n) = (4n^2-4nk+k^2-k)\psi_k^0(n) \quad \text{for} \quad \lambda_k^2 = -2k+6,\\
&\psi_k^3(n) = (8n^3-12n^2k+6nk^2-6nk+4n-k^3+3k^2-2k)\psi_k^0(n)\\
&\qquad \text{for} \quad \lambda_k^3 = -2k+8.
\end{aligned}$$

Moreover, the conditions in Equations (10)–(12) mean that we restrict the sequences $\{\psi_k^m\}$ to the spaces $\ell_k(\{k+1,k+2,\ldots\},\mathbb{C})$.

These expressions suggest to look for solutions of the eigenvalue problem in Equation (7) for a fixed k in the form

$$\psi_k^m(n) = P_k^m(n)\psi_k^0(n).$$

Substituting this expression into the difference equation (Equation (7)), after some calculations, we get the equation for the sequence $P_k^m(n)$:

$$(k-n)P_k^m(n+1) - kP_k^m(n) + nP_k^m(n-1) = (2-\lambda_k^m - 2k)\, P_k^m(n). \tag{16}$$

We recognize this as the equation for the Meixner polynomials (see [26]). Comparing Equations (16) and (2), we identify

$$\sigma(n) = n, \tag{17}$$
$$\tau(n) = k - 2n, \tag{18}$$
$$\lambda = \lambda_k^m + 2k - 2. \tag{19}$$

Finally, from the comparison of Equations (17)–(19) with Equations (3)–(5) under the condition $\lambda_k^m = \alpha_{k-m}$, we can see that P_k^m are the generalized Meixner polynomials of the first kind

$$P_k^m(n) = M_m^{-k,-1}(n).$$

To summarize the previous treatment, the eigenfunctions of the operators $\mathbf{H_k}$ are given by families of polynomials, which are indexed by the parameter k, with ground states such that

$$\mathbf{H_k} M_m^{-k,-1}(n)\psi_k^0(n) = 2(1-k+m)M_m^{-k,-1}(n)\psi_k^0(n).$$

From Equation (13) and restricting to the subspace $\ell_k(\{k+1,k+2,\dots\},\mathbb{C})$, we only get that

$$\left\langle \mathbf{A_k^*}\psi_{k-1}^0|\psi_k^0\right\rangle_k = \sum_{n=k}^{\infty} \overline{\psi_{k-1}^0(n)}\psi_k^0(n+1)\rho_{k-1}(n) +$$

$$+ \sum_{n=k+1}^{\infty} \overline{\psi_{k-1}^0(n)}\,(n-k)\,\psi_k^0(n)\rho_{k-1}(n) = \overline{\psi_{k-1}^0(k)}\psi_k^0(k+1)\rho_{k-1}(k),$$

because the function ψ_k^0 is not defined at the point k. This means that we have the following relationship $\langle\psi_k^1|\psi_k^0\rangle_k + \dfrac{1}{k!} = 0$, where we have put $C_k = 1$. Similarly, we obtain

$$\left\langle \psi_k^m|\psi_k^0\right\rangle_k - (-1)^m \frac{M_{m-1}^{-k+1,-1}(k)}{k!} = 0$$

for $m \geq 1$. In the language of the polynomials $M_m^{-k,-1}$, we can rewrite it in the form

$$\sum_{n=k+1}^{\infty} M_m^{-k,-1}(n)\frac{(-1)^{n+k}(n-k-1)!}{n!} - (-1)^m \frac{M_{m-1}^{-k+1,-1}(k)}{k!} = 0.$$

4. Conclusions

In this work, we propose a discrete version of the harmonic oscillator, which has a spectrum analogous to the corresponding problem in the continuous case. Our construction is based on a factorization method applied to second-order difference equations. In this case, the eigenfunctions turn out to be associated with the Meixner polynomials.

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