Physics Letters A 380 (2016) 68–75

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Exact discretization of Schrödinger equation

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ARTICLE INFO

Article history:
Received 10 August 2015
Received in revised form 21 September 2015
Accepted 23 October 2015
Available online 2 November 2015
Communicated by C.R. Doering

Keywords:
Quantum theory
Schrödinger equation
Difference
Discrete approximation
Long-range interaction

ABSTRACT

There are different approaches to discretization of the Schrödinger equation with some approximations. In this paper we derive a discrete equation that can be considered as exact discretization of the continuous Schrödinger equation. The proposed discrete equation is an equation with difference of integer order that is represented by infinite series. We suggest differences, which are characterized by power-law Fourier transforms. These differences can be considered as exact discrete analogs of derivatives of integer orders. Physically the suggested discrete equation describes a chain (or lattice) model with long-range interaction of power-law form. Mathematically it is a uniquely highlighted difference equation that exactly corresponds to the continuous Schrödinger equation. Using the Young's inequality for convolution, we prove that suggested differences are operators on the Hilbert space of square-summable sequences. We prove that the wave functions, which are exact discrete analogs of the free particle and harmonic oscillator solutions of the continuous Schrödinger equations, are solutions of the suggested discrete Schrödinger equations.

1. Introduction

The Schrödinger equation in coordinate representation is a partial differential equation that describes dynamics of pure quantum state of Hamiltonian quantum system [1]. In the general form of quantum theory, we should consider dynamics of non-Hamiltonian and open quantum systems, where quantum states are described by density operator [2]. The one-dimensional time-dependent Schrödinger equation in coordinate representation has the form

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2\mu}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\,\Psi(x,t), \tag{1}$$

where μ is the reduced mass, $V(x)$ is the potential energy, i is the imaginary unit, $\hbar$ is the Planck constant and $\Psi(x,t)$ is the wave function. Usually discretization of equation (1) is realized by using the standard central difference operator with the step a (for example, see [3,4]) for the second-order derivative

$$i\hbar \frac{d\Psi_n(t)}{dt} = -\frac{\hbar^2}{2\mu}\frac{1}{a^2}\Big(\Psi_{n+1}(t) - 2\Psi_n(t) + \Psi_{n-1}(t)\Big) + V_n\,\Psi_n(t), \tag{2}$$

where $\Psi_n(t) = \Psi(na,t)$. It is well-known that the finite difference of integer order n cannot be considered as an exact discretization of the derivative of this order [5]. For example, the central finite difference ${}^c\Delta_a^2$ of second order with step a can be represented [6] in the form

$${}^c\Delta_a^2 = 2\sum_{m=1}^{\infty} a^{2m}\,\frac{1}{(2m)!}\,\frac{\partial^{2m}}{\partial x^{2m}} \tag{3}$$

by using the well-known relations

$$\exp\left(a\frac{\partial}{\partial x}\right)\Psi(x,t) = \Psi(x+a,t). \tag{4}$$

There are various approaches to discretization of the Schrödinger equation with some approximations [4]. In this paper, we do not consider these approaches. We consider a problem of an exact discretization of the continuous Schrödinger equation. The problems of exact discretization have been formulated in [28–30]. Mickens proved that for differential equations there are "locally exact" finite-difference schemes, where the local truncation errors are zero. In this paper, we propose new approach that is based on new difference operators, which can be considered as an exact discretization of derivatives of integer orders. Using this approach, we get an exact discretization of the continuous Schrödinger equation. Our aim is a derivation of an exact discrete analogue of the Schrödinger equation. Using the Fourier transforms, we obtain a discrete equation that exactly corresponds to the continuous Schrödinger equation (1). The proposed discrete Schrödinger equation is equation with new difference of second order that has a power-law form of the Fourier transform. Physically this equation

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http://dx.doi.org/10.1016/j.physleta.2015.10.039

describes a model of chain or lattice with long-range interaction [7,8]. Mathematically it is uniquely given difference equation that exactly corresponds to the continuous Schrödinger equation. We prove not only an exact correspondence between the equations, but also an exact correspondence between solutions. We demonstrate that exact discrete analogs of the free particle and harmonic oscillator solutions of the continuous Schrödinger equation are solutions of the suggested difference equations in contrast to the situation with equations with the usual finite differences. For simplification, we will consider one-dimensional Schrödinger equation only. A generalization for three-dimensional case can be easily realized by the method proposed in [10,11].

2. From finite-difference equation to continuous Schrödinger equation

Let us give some details to prove that finite-difference equation (2) cannot exactly correspond to the continuous Schrödinger equation (1). For this aim we can use the Fourier series transform $\mathcal{F}_{a,\Delta}$ that is defined by the equation

$$\hat{\Psi}(k,t) = \mathcal{F}_{a,\Delta}\{\Psi_n(t)\} := \sum_{n=-\infty}^{+\infty} \Psi_n(t)\, e^{-ikna}. \tag{5}$$

Applying the transform $\mathcal{F}_{a,\Delta}$ to the finite-difference equation (2), we get

$$i\hbar \frac{d\hat{\Psi}(k,t)}{dt} = -\frac{\hbar^2}{2\mu} \sum_{m=1}^{\infty} \frac{2(-1)^m}{(2m)!\, a^2} (ka)^{2m}\, \hat{\Psi}(k,t) + (\hat{V} * \hat{\Psi})(k,t), \tag{6}$$

where $*$ denotes the convolution. The inverse Fourier integral transform $\mathcal{F}^{-1}$, which is defined by the equation

$$\Psi(x,t) = \mathcal{F}^{-1}\{\hat{\Psi}(k,t)\} := \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk\, \hat{\Psi}(k,t)\, e^{ikx}, \tag{7}$$

leads us to the fact that the inverse Fourier transform $\mathcal{F}^{-1}$ of equation (6) gives

$$i\hbar \frac{d\Psi(x,t)}{dt} = -\frac{\hbar^2}{2\mu} \sum_{m=1}^{\infty} \frac{2\, a^{2m-2}}{(2m)!} \frac{\partial^{2m}\Psi(x,t)}{\partial x^{2m}} + V(x)\, \Psi(x,t). \tag{8}$$

Equation (8) also can be obtained (for details, see Section 8 of [6]) by using the well-known relation (4). Equation (8) gives the Schrödinger equation (1) only in the limit $a \to 0$, where

$$\lim_{a\to 0} \sum_{m=1}^{\infty} \frac{2\, a^{2m-2}}{(2m)!} \frac{\partial^{2m}\Psi(x,t)}{\partial x^{2m}} = \frac{\partial^2 \Psi(x,t)}{\partial x^2}. \tag{9}$$

As a result, we proved that equation (2) can give equation (1) by deleting all terms $O(a^2)$ or by passing to the limit $a \to 0$ only. Therefore finite difference equation (2) cannot be considered as an exact discretization of (1).

The reason that equation (2) is an inexact (approximate) discretization of the Schrödinger equation (1) is the fact that the central finite difference ${}^{c}\Delta^2$ of second order is characterized by the inequality

$$\mathcal{F}_{a,\Delta}\left({}^{c}\Delta^2\right) \neq (ika)^2. \tag{10}$$

This inequality directly leads us (see equation (8)) to the corresponding inequality

$$\frac{1}{a^2}\mathcal{F}^{-1}\left(\mathcal{F}_{a,\Delta}\left({}^{c}\Delta^2\right)\right) \neq \frac{\partial^2}{\partial x^2}, \tag{11}$$

which means that this finite difference of second orders cannot give exactly the derivative of second order $\partial^2/\partial x^2$. Only in the limit $a \to 0$, we get

$$\lim_{a\to 0} \frac{\mathcal{F}^{-1}\left(\mathcal{F}_{a,\Delta}\left({}^{c}\Delta^2\right)\right)}{a^2} = \frac{\partial^2}{\partial x^2}. \tag{12}$$

Therefore the discrete equation (2) can be considered only as approximation of the Schrödinger equation (1). Finite difference equation (2) cannot be considered as an exact analogue of the Schrödinger equation (1).

3. Derivation of exact discrete Schrödinger equation from continuous equation

In the previous section, we prove that discrete equation (2) cannot be considered as an exact discretization of the Schrödinger equation (1). In this section, we derive new discrete Schrödinger equation from the continuous Schrödinger equation (1) by using the Fourier transforms.

To have an exact discrete analogue of the continuous Schrödinger equation (1), we should consider a problem of discretization of this equation in details. Let us consider a problem of derivation of an exact discrete analogue of the Schrödinger equation (1). To solve this problem, we should find new type of differences of integer order $n \in \mathbb{N}$, which will be denoted by ${}^{\mathcal{T}}\Delta^n$, that exactly correspond to the derivatives $\partial^n/\partial x^n$ with $n \in \mathbb{N}$. In order to the differences ${}^{\mathcal{T}}\Delta^n$ of orders $n \in \mathbb{N}$ correspond to the derivatives $\partial^n/\partial x^n$ exactly, these differences should satisfy the condition

$$\frac{1}{a^n}\mathcal{F}^{-1}\left(\mathcal{F}_{a,\Delta}\left({}^{\mathcal{T}}\Delta^n\, \Psi_m(t)\right)\right) = \frac{\partial^n \Psi(x,t)}{\partial x^n} \tag{13}$$

in contrast to the usual finite differences that are represented by infinite series of derivatives. Equation (13) can be considered as a characteristic property (criterion) of exact discretization.

Condition (13) can be realized if the difference ${}^{\mathcal{T}}\Delta^n$ has the Fourier series transform in the form

$$\mathcal{F}_{a,\Delta}\{{}^{\mathcal{T}}\mathbf{\Delta}^n\, \Psi_m(t)\} := \sum_{m=-\infty}^{+\infty} e^{-ikam}\, {}^{\mathcal{T}}\mathbf{\Delta}^n\, \Psi_m(t) = (ika)^n\, \hat{\Psi}(k,t) \tag{14}$$

In order to get (14), the differences ${}^{\mathcal{T}}\mathbf{\Delta}^\alpha$ of order $\alpha \in \mathbb{N}$ should be represented by the convolution

$$\begin{aligned} {}^{\mathcal{T}}\mathbf{\Delta}^\alpha\, \Psi_n(t) &:= \sum_{m=-\infty}^{+\infty} K_\alpha(m)\, \Psi_{n-m}(t) \\ &= \sum_{m=-\infty}^{+\infty} K_\alpha(n-m)\, \Psi_m(t) \quad (\alpha \in \mathbb{N}), \end{aligned} \tag{15}$$

where the kernels $K_\alpha(m)$ are characterized by the equations

$$\begin{aligned} &\mathcal{F}_{1,\Delta}\{K_{2s}(m)\} = (-1)^s\, k^{2s}, \\ &\mathcal{F}_{1,\Delta}\{K_{2s-1}(m)\} = -i\,(-1)^s\, k^{2s-1}, \quad (s \in \mathbb{N}) \end{aligned} \tag{16}$$

and

$$K_{2s}(-m) = K_{2s}(m), \quad K_{2s-1}(-m) = -K_{2s-1}(m) \tag{17}$$

that hold for all $s \in \mathbb{N}$ and $m \in \mathbb{Z}$.

Using (16) and (17), the kernels $K_\alpha(m)$ can be defined by the equations

$$K_{2s}(m) = \mathcal{F}^{-1}_{1,\Delta}\{(-1)^s k^{2s}\} = (-1)^s \frac{1}{\pi} \int_0^{\pi} k^{2s} \cos(km)\, dk, \tag{18}$$

$$K_{2s-1}(m) = \mathcal{F}^{-1}_{1,\Delta}\{-i\,(-1)^s k^{2s-1}\} = (-1)^s \frac{1}{\pi} \int_0^{\pi} k^{2s-1} \sin(km)\, dk. \tag{19}$$

Using equation 2.5.3.5 of [9], we obtain

$$K_{2s}(m) = \sum_{k=0}^{s-1} \frac{(-1)^{m+k+s}\,(2s)!\,\pi^{2s-2k-2}}{(2s-2k-1)!} \frac{1}{m^{2k+2}} \quad (m \in \mathbb{Z}, \quad m \neq 0), \tag{20}$$

$$K_{2s-1}(m) = \sum_{k=0}^{s-1} \frac{(-1)^{m+k+s+1}\,(2s-1)!\,\pi^{2s-2k-2}}{(2s-2k-1)!} \frac{1}{m^{2k+1}} \quad (m \in \mathbb{Z}, \quad m \neq 0), \tag{21}$$

and

$$K_{2s}(0) = \frac{(-1)^s \pi^{2s}}{2s+1}, \quad K_{2s-1}(0) = 0. \tag{22}$$

As a result, we obtain that $\mathcal{T}$-differences are defined by equations (15) with the kernels (20)–(22). Let us give examples of the suggested $\mathcal{T}$-differences of orders $\alpha = 1, 2, 3, 4$.

The $\mathcal{T}$-difference of first order has the form

$$^{\mathcal{T}}\mathbf{\Delta}^1\, \Psi_n(t) := \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \frac{(-1)^m}{m}\, \Psi_{n-m}(t). \tag{23}$$

The $\mathcal{T}$-difference of second order has the form

$$^{\mathcal{T}}\mathbf{\Delta}^2\, \Psi_n(t) := -\sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \frac{2\,(-1)^m}{m^2}\, \Psi_{n-m}(t) - \frac{\pi^2}{3}\, \Psi_n(t). \tag{24}$$

The $\mathcal{T}$-difference of third order is

$$^{\mathcal{T}}\mathbf{\Delta}^3\, \Psi_n(t) := -\sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \left(\frac{(-1)^m \pi^2}{m} - \frac{6\,(-1)^m}{m^3} \right) \Psi_{n-m}(t). \tag{25}$$

The $\mathcal{T}$-difference of fourth order is

$$^{\mathcal{T}}\mathbf{\Delta}^4\, \Psi_n(t) := \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \left(\frac{4\pi^2\,(-1)^m}{m^2} - \frac{24\,(-1)^m}{m^4} \right) \Psi_{n-m}(t) + \frac{\pi^4}{5}\, \Psi_n(t). \tag{26}$$

Using the suggested $\mathcal{T}$-differences, we can consider the following discretization. Starting from the continuous Schrödinger equation (1), we obtain an exact discrete analogue of this continuous Schrödinger equation without approximation, which is based on deleting the terms $O(a^2)$ or on the passing to the limit $a \to 0$.

Let us find an exact analogue of the Schrödinger equation. For this aim, we use the Fourier integral transform $\mathcal{F}$, which is defined by equation

$$\hat{\Psi}(k,t) := \mathcal{F}\{\Psi(x,t)\} = \int_{-\infty}^{+\infty} dx\, \Psi(x,t)\, e^{-ikx}. \tag{27}$$

Applying this Fourier transform to the Schrödinger equation (1), we get

$$i\hbar \frac{\partial \hat{\Psi}(k,t)}{\partial t} = \frac{\hbar^2}{2\mu} k^2\, \hat{\Psi}(k,t) + (\hat{V} * \hat{\Psi})(k,t), \tag{28}$$

where $*$ denotes the convolution. Using the inverse Fourier series transform

$$\Psi_n(t) := \mathcal{F}^{-1}_{a,\Delta}\{\hat{\Psi}(k,t)\} = \frac{a}{2\pi} \int_{-\pi/a}^{+\pi/a} dk\, \hat{\Psi}(k,t)\, e^{ikna}, \tag{29}$$

equation (28) gives

$$i\hbar \frac{d\Psi_n(t)}{dt} = -\frac{\hbar^2}{2\mu} \frac{1}{a^2}\, {}^{\mathcal{T}}\mathbf{\Delta}^2\, \Psi_n(t) + V_n\, \Psi_n(t), \tag{30}$$

where ${}^{\mathcal{T}}\mathbf{\Delta}^2$ is the $\mathcal{T}$-difference of second order that is defined by equation (24). Substituting (24) into (30), we obtain

$$i\hbar \frac{d\Psi_n(t)}{dt} = \frac{\hbar^2}{2\mu} \frac{2}{a^2} \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \frac{(-1)^m}{m^2}\, \Psi_{n-m}(t) + \frac{\hbar^2}{2\mu} \frac{\pi^2}{3a^2}\, \Psi_n(t) + V_n\, \Psi_n(t). \tag{31}$$

As a result, we derive the exact discrete analogue of the continuous time-dependent Schrödinger equation (1) in the form of the $\mathcal{T}$-difference equation (31). The discrete Schrödinger equation (31) is the result of exact discretization of the continuous time-dependent equation (1). Note that the suggested discretization of the Schrödinger equation is exact for wide class of potentials. In the next sections, we demonstrate that discrete analogs of solutions of the continuous Schrödinger equation (1) can be solutions of the suggested discrete equation (31).

4. Mathematical remarks and Hilbert space

In this section, we give some mathematical remarks about the suggested $\mathcal{T}$-difference Schrödinger equation (30).

In quantum mechanics the discrete wave-function $\Psi_n(t)$ should belong to the Hilbert space l^2 of square-summable sequences for all $t \geq 0$. In addition, to use the Fourier series transform, we also should assume that the function $\Psi_n(t)$ belongs to the Hilbert space l^2, where the norm on the l^p-space is defined by the equation

$$\|\Psi\|_p := \left(\sum_{n=-\infty}^{+\infty} |\Psi_n|^p \right)^{1/p}.$$

It is easy to see that the $\mathcal{T}$-differences (24) and (15) with (20) are defined by convolutions of $\Psi_m(t) \in l^2$ and the functions

$$a_{2n}(m) = \frac{(-1)^m}{m^{2n}} \quad (m \neq 0, \quad m \in \mathbb{Z}, \quad n \in \mathbb{N})$$

that belong to the space l^1. Using the Young's inequality for convolution (see [16,17] and Theorem 276 of [18]) in the form

$$\|\, {}^{\mathcal{T}}\mathbf{\Delta}^{2n}\, \Psi\|_r = \|a_{2n} * \Psi\|_r \leq \|a_{2n}\|_p\, \|\Psi\|_q, \tag{32}$$

where

$$\frac{1}{r} + 1 = \frac{1}{p} + \frac{1}{q}, \tag{33}$$

we get that $r = 2$ and the result of the action of operators ${}^{\mathcal{T}}\mathbf{\Delta}^{2n}$ on the function $\Psi_n \in l^2$ also belongs to the Hilbert space l^2 of square-summable sequences, i.e.

$${}^{\mathcal{T}}\mathbf{\Delta}^{2n}\, \Psi_m \in l^2, \tag{34}$$

since condition (33) holds. As a result, the $\mathcal{T}$-differences are the operators on the Hilbert space l^2 of square-summable sequences, i.e. ${}^{\mathcal{T}}\mathbf{\Delta}^{2n} : l^2 \to l^2$.

Note that using equation 5.1.2.3 of [9], we can get

$$\sum_{m=1}^{\infty} K_{2n}(m) = \sum_{m=1}^{\infty} \frac{2(-1)^m}{m^{2n}} = 2\,(2^{1-2n} - 1)\,\zeta(2n)$$
$$= -\frac{2}{\Gamma(2n)} \int_0^{\infty} \frac{x^{2n-1}}{e^x + 1} dx = 2\,T_{2n}, \qquad (35)$$

where $\zeta(z)$ is the Riemann zeta function, $\Gamma(z)$ is the Gamma function. For example, we have

$$T_2 = -\frac{\pi^2}{12}, \quad T_4 = -\frac{7\pi^4}{720},$$
$$T_6 = -\frac{31\pi^6}{32 \cdot 945}, \quad T_8 = -\frac{127\pi^8}{128 \cdot 9450}.$$

As a result, the $\mathcal{T}$-differences acting on constant converge to zero (${}^{\mathcal{T}}\mathbf{\Delta}^{2n}\,\mathrm{const} = 0$).

The main property of the suggested differences is that the Fourier series transform $\mathcal{F}_{a,\Delta}$ is represented by the equality

$$\mathcal{F}_{a,\Delta}\left({}^{\mathcal{T}}\mathbf{\Delta}^n\right) = (i\,k\,a)^n, \qquad (36)$$

in contrast to equation (11) for finite difference. Equation (36) leads us to the corresponding equality

$$\frac{1}{a^n}\mathcal{F}^{-1}\left(\mathcal{F}_{a,\Delta}\left({}^{\mathcal{T}}\mathbf{\Delta}^n\right)\right) = \frac{1}{a^n}\mathcal{F}^{-1}\left((i\,k\,a)^n\right) = \frac{\partial^n}{\partial x^n}, \qquad (37)$$

which means that this difference ${}^{\mathcal{T}}\mathbf{\Delta}^n$ of order n gives the derivative $\partial^n/\partial x^n$ exactly. We see that these $\mathcal{T}$-differences of orders n are connected with the derivatives $\partial^n/\partial x^n$ without deleting all terms $O(a^2)$ and passing to the limit $a \to 0$. The limit $a \to 0$ also gives exactly the derivatives

$$\lim_{a \to 0} \frac{\mathcal{F}^{-1}\left(\mathcal{F}_{a,\Delta}\left({}^{\mathcal{T}}\mathbf{\Delta}^n\right)\right)}{a^n} = \frac{\partial^n}{\partial x^n}. \qquad (38)$$

As a result the suggested discrete Schrödinger equation (30) with $\mathcal{T}$-difference can be considered as an exact discretization of the continuous Schrödinger equation (1).

5. Discrete time-independent Schrödinger equations and free particle solution

In this section we compare the time-independent Schrödinger equation with finite difference and equation with the $\mathcal{T}$-difference.

Substitution of the wave function of the form $\Psi_n(t) = \Psi_n\, e^{-i\,E\,t/\hbar}$ into equation (30) with $a = 1$ gives the time-independent Schrödinger equation

$${}^{\mathcal{T}}\mathbf{\Delta}^2\,\Psi_n + \frac{2\,\mu}{\hbar^2}\,(E - V_n)\,\Psi_n = 0. \qquad (39)$$

Substitution of (24) into (39) gives

$$-\sum_{\substack{m=-\infty \\ m \neq 0}}^{+\infty} \frac{2\,(-1)^m}{m^2}\,\Psi_{n-m} + \left(\frac{2\,\mu}{\hbar^2}\,(E - V_n) - \frac{\pi^2}{3}\right)\Psi_n = 0. \qquad (40)$$

In the suggested $\mathcal{T}$-difference approach to discretization, equation (40) is the eigenvalue equation for infinite matrix. As a result, the time-independent Schrödinger equation leads to an eigenvalue problem for infinite matrices [12–15].

Let us consider the free particle solution of the discrete time-independent Schrödinger equations with finite and $\mathcal{T}$ differences. Free particle is a particle that has no external forces acting upon it, in other words the potential energy is constant $V_n = U_0 = \mathrm{const}$. In this case, the discrete time-independent Schrödinger equation with $\mathcal{T}$-difference has the form

$${}^{\mathcal{T}}\mathbf{\Delta}^2\,\Psi_n + k^2\,\Psi_n = 0, \qquad (41)$$

where ${}^{\mathcal{T}}\mathbf{\Delta}^2$ is defined by (24) with $a = 1$, and

$$k = \frac{1}{\hbar}\sqrt{2\,\mu\,(E - U_0)}. \qquad (42)$$

The discretization of equation (1) by the central difference has the form

$${}^{c}\Delta^2\,\Psi_n + k^2\,\Psi_n = 0, \qquad (43)$$

where ${}^{c}\Delta^2$ is the central finite difference of second order with the step $a = 1$. Let us compare solutions of equations (41) and (43) that can be written in the form

$$-\sum_{\substack{m=-\infty \\ m \neq 0}}^{+\infty} \frac{2\,(-1)^m}{m^2}\,\Psi_{n-m} - \frac{\pi^2}{3}\,\Psi_n + k^2\,\Psi_n = 0, \qquad (44)$$

and

$$\Psi_{n-1} - 2\,\Psi_n + \Psi_{n-1} + k^2\,\Psi_n = 0, \qquad (45)$$

for the differences ${}^{\mathcal{T}}\mathbf{\Delta}^2$ and ${}^{c}\Delta^2$, respectively.

Let us consider the wave functions of the form

$$\Psi_n = a\,\cos(k\,n) + b\,\sin(k\,n) = A\,\cos\Big(k\,n + \phi_0\Big), \qquad (46)$$

which is an exact discrete analogue of the solution $\Psi(x) = A\,\cos(k\,x + \phi_0)$ of the continuous time-independent Schrödinger equation.

Let us consider (46) for the finite-difference Schrödinger equation (45). For central finite difference, we can use the formula that expresses the cosine of sums of angles. Then the central difference gives

$${}^{c}\Delta^2\,\cos\Big(k\,n + \phi_0\Big) = 2\,\cos\Big(k\,n + \phi_0\Big)\Big(\cos(k) - 1\Big) =$$
$$= -k^2\,\cos\Big(k\,n + \phi_0\Big) - \sum_{n=1}^{\infty} \frac{2\,(-1)^n}{(2n)!}\,k^{2n}\,\cos\Big(k\,n + \phi_0\Big). \qquad (47)$$

It is easy to see that

$${}^{c}\Delta^2\,\cos\Big(k\,n + \phi_0\Big) \neq -k^2\,\cos\Big(k\,n + \phi_0\Big).$$

Substitution of (47) into equation (45) cannot give the equality. As a result, we get that the wave function (46), which is an exact discrete analogue of the solution of the continuous Schrödinger equation, cannot be a solution of the finite-difference Schrödinger equation (45). Therefore equation (45) cannot be considered as an exact discretization of the continuous Schrödinger equation. Equation (45) is discretization with an approximation.

Let us consider (46) for the $\mathcal{T}$-difference Schrödinger equation (44). Using the relations

$$\sum_{\substack{m=-\infty \\ m \neq 0}}^{+\infty} \frac{2\,(-1)^m}{m^2}\,\Psi_{n-m} = \sum_{m=1}^{+\infty} \frac{2\,(-1)^m}{m^2}\,(\Psi_{n-m} + \Psi_{n+m}) \qquad (48)$$

and

$$\cos\Big(k\,(n - m) + \phi_0\Big) + \cos\Big(k\,(n + m) + \phi_0\Big)$$
$$= 2\,\cos\Big(k\,n + \phi_0\Big)\,\cos(k\,m), \qquad (49)$$

we get the equation for the $\mathcal{T}$-difference

$$ {}^{\mathcal{T}}\mathbf{\Delta}^2 \cos\Big(kn+\phi_0\Big) = -4\cos\Big(kn+\phi_0\Big) \sum_{m=1}^{+\infty} \frac{(-1)^m}{m^2} \cos(km) - \frac{\pi^2}{3} \cos\Big(kn+\phi_0\Big). \quad (50) $$

Applying equation 5.4.2.8 or 5.4.2.12 of [9] in the form

$$ \sum_{m=1}^{+\infty} \frac{(-1)^m}{m^2} \cos(km) = \frac{1}{12}(3k^2-\pi^2) \quad (-\pi \le k \le \pi), \quad (51) $$

we get that equation (50) takes the form

$$ {}^{\mathcal{T}}\mathbf{\Delta}^2 \cos\Big(kn+\phi_0\Big) = -4\cos\Big(kn+\phi_0\Big) \left(\frac{1}{4}k^2 - \frac{\pi^2}{12}\right) - \frac{\pi^2}{3} \cos\Big(kn+\phi_0\Big). \quad (52) $$

As a result, we obtain the equation

$$ {}^{\mathcal{T}}\mathbf{\Delta}^2 \cos\Big(kn+\phi_0\Big) = -k^2 \cos\Big(kn+\phi_0\Big). \quad (53) $$

Note that this equation is an exact discrete analogue of the equation $(\cos(kx))'' = -k^2\cos(kx)$.

Substitution of (53) into equation (44) gives the equality. As a result, we get that the wave function (46) is a solution of the $\mathcal{T}$-difference Schrödinger equation (44). We prove that the wave function (46), which is an exact discrete analogue of the solution of the continuous Schrödinger equation, is a solution of the suggested discrete Schrödinger equation (44). This demonstrates that equation (44) can be considered as an exact discretization of the continuous Schrödinger equation (1).

6. Discrete time-independent Schrödinger equations of quantum harmonic oscillator

Let us compare the time-independent Schrödinger equation with finite difference and the suggested $\mathcal{T}$ difference for quantum harmonic oscillator.

In coordinate representation, the time-independent Schrödinger equation of harmonic oscillator has the form

$$ -\frac{\hbar^2}{2\mu}\frac{d^2\Psi(x)}{dx^2} + \left(\frac{\mu\omega^2 x^2}{2} - E\right)\Psi(x) = 0, \quad (54) $$

where E denotes real number that is a time-independent energy, ω is the angular frequency of the oscillator. Using the variables

$$ z = \frac{x}{x_0}, \quad x_0 = \sqrt{\frac{\hbar}{\mu\omega}}, \quad \lambda = \frac{2E}{\hbar\omega}, \quad (55) $$

equation (54) can be represented in the form

$$ \frac{d^2\Psi(x)}{dx^2} + \Big(\lambda - z^2\Big)\Psi(x) = 0, \quad (56) $$

where λ is the positive real parameter.

The exact discrete analog of the Schrödinger equation (56) is the $\mathcal{T}$-difference equation of the form

$$ {}^{\mathcal{T}}\mathbf{\Delta}^2 \Psi_n + (\lambda - n^2)\Psi_n = 0. \quad (57) $$

We will seek a solution Ψ_n of equation (57) that belongs to the Hilbert space l^2 in the form

$$ \Psi_n = g[n]\exp[-n^2/2]. \quad (58) $$

Note that $\exp[-n^2/2] \in l^2$, since

$$ \sum_{n=-\infty}^{+\infty} |\exp[-n^2/2]|^2 = \theta_3(0, 1/e) < \infty, \quad (59) $$

where $\theta_3(z,q)$ is the Jacobi theta-functions.

Let us substitute (58) into (57). Then the Leibniz rule for $\mathcal{T}$-difference of first order

$$ {}^{\mathcal{T}}\mathbf{\Delta}^1 \Big(g[n]\exp[-n^2/2]\Big) = g[n]\,{}^{\mathcal{T}}\mathbf{\Delta}^1 \exp[-n^2/2] + \exp[-n^2/2]\,{}^{\mathcal{T}}\mathbf{\Delta}^1 g[n], \quad (60) $$

and the equation

$$ {}^{\mathcal{T}}\mathbf{\Delta}^1 \exp[-n^2/2] = -n\exp[-n^2/2], \quad (61) $$

which are proved by the Taylor series and the formula of difference of power-law function, give the equation for the function $g[n]$ in the form

$$ {}^{\mathcal{T}}\mathbf{\Delta}^2 g[n] - 2n\,{}^{\mathcal{T}}\mathbf{\Delta}^1 g[n] + (\lambda-1)g[n] = 0. \quad (62) $$

To solve difference equation (62), we use the method of power series. Let us assume that

$$ g[n] = \sum_{k=0}^{\infty} a_k n^k. \quad (63) $$

Substitution of (63) into (62), gives

$$ \sum_{k=0}^{\infty} a_k\,{}^{\mathcal{T}}\mathbf{\Delta}^2 n^k - 2n\sum_{k=0}^{\infty} a_k\,{}^{\mathcal{T}}\mathbf{\Delta}^1 n^k + (\lambda-1)\sum_{k=0}^{\infty} a_k n^k = 0. \quad (64) $$

Then we can use the following equations of $\mathcal{T}$-difference of power-law functions

$$ {}^{\mathcal{T}}\mathbf{\Delta}^1 n^k = k n^{k-1}, \quad (k \ge 1), $$

$$ {}^{\mathcal{T}}\mathbf{\Delta}^2 n^k = k(k-1)n^{k-2}, \quad (k \ge 2) \quad (65) $$

$$ {}^{\mathcal{T}}\mathbf{\Delta}^m n^k = 0, \quad (k < m, \quad k, m \in \mathbb{N}), \quad (66) $$

which are proved by the Cesaro and Poisson–Abel summations [24–27] that give the expressions

$$ \sum_{m=1}^{+\infty} (-1)^m = -\frac{1}{2}, \quad \sum_{m=1}^{+\infty} (-1)^m m^{2j} = 0 \quad (j \in \mathbb{N}). \quad (67) $$

Then equation (64) has the form

$$ \sum_{k=0}^{\infty}\Big(a_k k(k-1)n^{k-2} - 2n a_k k n^{k-1} + (\lambda-1)a_k n^k\Big) = 0. \quad (68) $$

Changing the variable $k \to k+2$ of the first term and assuming $a_{-1} = a_{-2} = 0$, equation (68) can be written in the form

$$ \sum_{k=0}^{\infty}\Big(a_{k+2}(k+2)(k+1) - a_k(2k-\lambda+1)\Big)n^k = 0. \quad (69) $$

In order condition (69) to hold for all $n \in \mathbb{Z}$, we should have the equality

$$ a_{k+2} = a_k \frac{2k-\lambda+1}{(k+2)(k+1)}. \quad (70) $$

Using the recurrence relation (70), we can see that $\lim_{n\to\pm\infty}|\Psi_n| = \infty$. To obtain a solution $\Psi_n \in l^2$, we assume that there exists an integer number $N \in \mathbb{N}$ such that $a_k = 0$ for all $k > N$. In this case, the condition (70) gives $\lambda = 2N+1$, and equation (70) has the form

$$ a_{k+2} = a_k \frac{2(k-N)}{(k+2)(k+1)}. \quad (71) $$

In this case, we get that $g[n]$ is the discrete "physicists" Hermite polynomial of degree N and integer variable $g[n] = H^{ph}_N[n]$. It should be noted that the discrete "physicists" Hermite polynomials can be defined by the equation

$$H^{ph}_N[n] := (-1)^N e^{n^2}\, {}^{\mathcal{T}}\mathbf{\Delta}^N e^{-n^2}. \tag{72}$$

As a result, the wave-function

$$\Psi_{n,N} = A_N\, H^{ph}_N[n] \exp[-n^2/2] \quad (n \in \mathbb{Z}), \tag{73}$$

which is a solution of the Schrödinger $\mathcal{T}$-difference equation (58) that belongs to the Hilbert space l^2 of square summable sequences, where A_N is the normalization factor.

It should be noted that equation (73) defines the well-known exact discrete analog of the wave function of the harmonic oscillator. Solution (73) is similar to the solution $\Psi_N(x) = A_N \exp(-x^2/2)\, H_N(x)$ of the continuous Schrödinger equation (56).

Let us consider a discretization of the equation (56) by usual finite differences. For example, the discrete Schrödinger equation with forward difference has the form

$${}^f\Delta^2\, \Psi_n + (\lambda - n^2)\, \Psi_n = 0. \tag{74}$$

This equation cannot have a solution that is similar to (73), which is discrete analog of $\Psi_N(x) = A_N \exp(-x^2/2)\, H_N(x)$, since the Leibniz rule is not performed for the forward difference, i.e., we have the inequality

$$\begin{aligned} &{}^f\Delta^1 \Big(g[n] \exp[-n^2/2]\Big) \\ &\neq g[n]\, {}^f\Delta^1 \exp[-n^2/2] + \exp[-n^2/2]\, {}^f\Delta^1\, g[n], \end{aligned} \tag{75}$$

and since the differences of power-law functions n^k do not have the form (65),

$${}^f\Delta\, n^k = (n+1)^k - n^k = k\, n^{k-1} + \sum_{j=2}^{k} \binom{k}{j} n^j \neq k\, n^{k-1}. \tag{76}$$

It is easy to check that the equation with finite differences

$${}^f\Delta^2\, g[n] - 2n\, {}^f\Delta^1\, g[n] + (\lambda - 1)\, g[n] = 0 \tag{77}$$

cannot give a solution in the form of the discrete Hermite polynomials $H_N[n]$ by the method of power series, since we have inequality (76).

As a result, we get that the wave function (73) is a solution of the $\mathcal{T}$-difference Schrödinger equation. We proved that the wave function (73), which is an exact discrete analogue of the solution of the continuous Schrödinger equation (56), is a solution of the suggested discrete Schrödinger equation (44). This demonstrates that equation (57) can be considered as an exact discretization of the continuous Schrödinger equation. The Schrödinger equation with forward differences cannot be considered as an exact discretization of the continuous Schrödinger equation.

It should be noted that there is another type of exact discretization that is based on an approach suggested in [28–30]. For example, an exact discretization of the classical harmonic oscillator has been proposed [31,32]. This approach means that for each new equation, we should use new difference operators. Our approach is based on $\mathcal{T}$-differences ${}^{\mathcal{T}}\mathbf{\Delta}^n$, which can be considered as exact discretizations of derivatives $\partial^n/\partial x^n$. The suggested differences are represented by infinite series instead of finite series that are usually used in other difference approaches. The suggested discretization of the Schrödinger equation is exact for wide class of potentials. We demonstrate that discrete analogs of solutions of the continuous Schrödinger equation (1) can be solutions of the corresponding discrete equation (31).

7. Physical remarks and long-range interactions

In this section, we give remarks about direct connection of the suggested $\mathcal{T}$-differences and chain (and lattice) models with long-range interactions. We can state that the suggested discrete Schrödinger equation (30) with $\mathcal{T}$-differences corresponds to chain and lattice models with long-range interactions.

The main part of the previous discretizations of the Schrödinger equation is based on the forward, backward and central finite differences. These discretizations assume a short ranged and a nearest-neighbor approximation. However, there exist physical situations that cannot be described in the framework of this approximation. For example, the excitation transfer in molecular crystals [33] and the vibron energy transport in polymers [34] are due to the transition dipole–dipole interaction that corresponds to $K(n-m) = 1/|n-m|^3$. The DNA molecule contains charged groups with a long-range Coulomb interaction that corresponds to $K(n-m) = 1/|n-m|^1$ between them. In systems, where the dispersion curves of two elementary excitations are close or intersect, we have an effective long-range transfer. Such a situation arises for excitons and photons in molecular crystals and semiconductors, and it is called the polariton effects [33].

The well-known discrete nonlinear Schrödinger equation (DNLSE) for one-dimensional case has the form

$$i\hbar \frac{d\Psi_n(t)}{dt} = g \sum_{m=-\infty}^{+\infty} K_\alpha(n-m)\, \Psi_m(t) + F(\Psi_n(t)), \tag{78}$$

where g is a coupling constant, $F(\Psi_n)$ is an interaction of the particles with the external on-site force, $K_\alpha(n-m)$ is the kernel of the dispersive long-range interaction. The most famous type of long-range interaction [47,49–51,48,53] is given by

$$K_\alpha(n-m) = \frac{1}{|n-m|^\alpha} \quad (n, m \in \mathbb{Z}), \tag{79}$$

where α is a positive real number. In this case, we have nonlocal coupling given by the power-law function (79) with a physical relevant parameter α. Some integer values of α correspond to the well-known physical situations. For example, the Coulomb potential corresponds to $\alpha = 1$ and the dipole–dipole interaction corresponds to $\alpha = 3$.

Classical and quantum systems with long-range interactions are the subject of continuing interest in physics beginning with the works of Dyson [35,36] in 1969, where the interaction kernels of the form (79) are used. The long-range interactions have been studied in discrete systems as well as in their continuous analogues. Models of spins with long-range interactions have been studied in [35–43]. An infinite one-dimensional Ising model with long-range interactions is described by Dyson [35–37]. The d-dimensional classical Heisenberg model with long-range interaction is considered in [42], and its quantum generalization has been suggested in [38–41]. Kinks in lattice models with long-range particle interactions are studied in [52]. The breathers, which are time periodic spatially localized solutions, on discrete chains in the presence of long-range interactions are considered in [44–46]. Energy and decay properties of discrete breathers in systems with long-range interactions have also been studied in the framework of the discrete nonlinear Schrödinger equations [47,49–51,48,53,54]. The synchronization and dynamical chaos in chain models with long-range interaction of the form $1/|n|^\alpha$ are described in [58,56,55]. A remarkable property of the dynamics described by the lattice models with power-like long-range interactions is that the solutions have power-like tails [44,46,55–58]. Similar features were observed in continuous models that are described by differential equations with derivatives of non-integer orders. As it was shown in [7,8,10,11], the equations with fractional derivatives are directly related to chain and lattice models with long-range interactions.

If we consider the kernels $K_\alpha(n-m)$ in the form (20) and (21), which can be considered as linear combinations of the kernels (79), then equation (78) takes the form

$$i\hbar \frac{d\Psi_n(t)}{dt} = g^{\mathcal{T}} \mathbf{\Delta}^\alpha \Psi_m(t) + F(\Psi_n(t)), \quad (\alpha \in \mathbb{N}). \tag{80}$$

This is a discrete nonlinear Schrödinger equation with long-range interactions in the form of $\mathcal{T}$-differences.

It should be noted that the kernels (20) and (21) of the suggested $\mathcal{T}$-differences can be considered as linear combinations of kernels (79) with integer $\alpha \in \mathbb{N}$. The linear combinations (20) and (21) are selected from the set of other combinations by the fact that they exactly correspond to the local continuous systems, which are described by differential equations of integer orders. The suggested type of long-range interactions, which are described by the kernels (20) and (21) of $\mathcal{T}$-differences, is distinguished from others by exact discretization of corresponding differential equation of integer order and by preservation of the main (characteristic) properties of differential equations and corresponding solutions.

It should be noted that computer simulations are actively used for the linear and nonlinear systems with long-range interactions of the form (79) with integer and non-integer α (for example, see [47,49–51,46,53,57,58]). It allows us assume that computer simulations of equations with the suggested $\mathcal{T}$-differences, which are defined by the kernels (20) and (21), can be successfully realized since these kernels can be represented by linear combinations of (79) with $\alpha \in \mathbb{N}$. We assume that the discrete nonlinear Schrödinger equations with $\mathcal{T}$-differences can demonstrate new effects such as discrete kinks, solitons, breathers, synchronization and chaos by computer simulations.

8. Conclusion

In this paper, we suggest a discrete equation that corresponds to the continuous Schrödinger equation exactly. From a mathematical point of view, these discrete equations are uniquely highlighted equations with differences that exactly correspond to the Schrödinger equations. Physically the discrete equations describe microstructural models of chains (lattices) with long-range interactions. The main advantage of the suggested discrete equations is the connection with continuum equations without any approximation. We also prove that suggested differences are operators on the Hilbert space of square-summable sequences. It has been proved that an exact discrete analogue of the free particle solution of the continuous Schrödinger equation, is a solution of the suggested discrete Schrödinger equation. For simplification, we consider one-dimensional equations only. A generalization for three-dimensional case can be easily realized by the approach proposed in [10,11]. We assume that the suggested difference equations can be important in application since this allows us to reflect characteristic properties of complex systems and media [19–22] at the micro- and nano-scale, where long-range interactions play a crucial role in determining the properties of these systems (see [23] and references therein). For relativistic quantum theories, we assume that the proposed exact discretization approach can take into account the corresponding relativistic covariance by the methods considered in [22].

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