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Article

Exact Discrete Analogs of Canonical Commutation and Uncertainty Relations

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Abstract: An exact discretization of the canonical commutation and corresponding uncertainty relations are suggested. We prove that the canonical commutation relations of discrete quantum mechanics, which is based on standard finite difference, holds for constant wave functions only. In this paper, we use the recently proposed exact discretization of derivatives, which is based on differences that are represented by infinite series. This new mathematical tool allows us to build sensible discrete quantum mechanics based on the suggested differences and includes the correct canonical commutation and uncertainty relations.

Keywords: quantum theory; canonical commutation relation; uncertainty relations; exact discretization; finite difference

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1. Introduction

In the coordinate representation of quantum mechanics, the quantum observables are given by differential operators. The pure quantum states are described by wave functions. Dynamics of Hamiltonian quantum systems are represented by the Schrödinger equation that describes evolution of pure states of Hamiltonian quantum systems [1]. In the general case, we should consider dynamics of non-Hamiltonian and open quantum systems, where quantum states are represented by density operator and dynamics is described by quantum Markovian master equations [2], or non-Markovian master equations [3,4], where the memory effects are taken into account. Discretization of quantum mechanics is usually realized by using the standard finite differences [5]. It is well-known that finite differences cannot be considered as exact discrete analogues of differential operators. Therefore, the finite-difference discretization of the quantum mechanics can be considered only as an approximation. Strictly speaking, this discretization can lead to the violation of some fundamental relations of quantum mechanics such as canonical commutation relations. In order to consider an uncertainty relation of discrete quantum mechanics, we should have a correct discrete representation of the Heisenberg canonical commutation relations.

In this paper, we prove that the canonical commutation relation of the discrete quantum mechanics, which is based on standard finite differences, holds only for constant wave functions. To get a correct uncertainty relation of discrete quantum mechanics, we propose an exact discretization of the canonical commutation relations. In this paper, we use the recently suggested lattice calculus [6–8] and approach to exact discretization [9–12], which is based on new type differences. This new mathematical tool allows us to build sensible and consistent discrete quantum mechanics by using the proposed $\mathcal{T}$-differences of integer orders [9,10]. We give the proofs of the discrete analogs of the canonical commutation and uncertainty relations. For simplification, we will consider only the one-dimensional coordinate representation of quantum mechanics.

2. Canonical Commutation Relations with Standard Finite Differences

In order to consider an uncertainty relation of discrete quantum mechanics, we should have the correct Heisenberg canonical commutation relations. In this section, we prove that standard differences cannot be used to achieve this aim.

In the coordinate representation, the coordinate and momentum operators are defined by the equations:

$$\hat{q}\,\Psi(x) = x\,\Psi(x) \tag{1}$$

$$\hat{p}\,\Psi(x) = -\,i\,\hbar\,\frac{d}{dx}\,\Psi(x) \tag{2}$$

where $\Psi(x)$ is the wave function and $\hbar$ is the Planck constant.

Using the forward finite difference to discretize the first-order derivative, we can write

$$\hat{p}\,\Psi[n] = -\,i\,\hbar\,{}^{f}\Delta^{1}\,\Psi[n] \tag{3}$$

where $\Psi[n]$ is a discrete analog of the wave function $\Psi(x)$ (for example, $\Psi[n] = h\Psi(hn)$, where $h > 0$ is the step of discretization [10]), and ${}^{f}\Delta^{1}$ is the forward finite difference of first order that is defined in the form:

$${}^{f}\Delta^{1}\,\Psi[n] := \Psi[n+1] - \Psi[n] \tag{4}$$

Using Equation (3) and $\hat{q}\,\Psi[n] = n\,\Psi[n]$, the canonical commutation relation,

$$\hat{q}\,\hat{p}\,\Psi[n] - \hat{p}\,\hat{q}\Psi[n] = i\,\hbar\,\Psi[n] \tag{5}$$

is represented by the forward finite difference equation,

$$-\,i\,\hbar\,\Big(n\,{}^{f}\Delta^{1}\,\Psi[n] - {}^{f}\Delta^{1}\,(n\,\Psi[n])\Big) = i\,\hbar\,\Psi[n] \quad (for\ all\ n \in \mathbb{Z}) \tag{6}$$

Using Equations (4) and (6) takes the form:

$$-\,i\,\hbar\,\Big(n\,(\Psi[n+1] - \Psi[n]) - ((n+1)\,\Psi[n+1] - n\,\Psi[n])\Big) = i\,\hbar\,\Psi[n] \quad (for\ all\ n \in \mathbb{Z}) \tag{7}$$

Removing the small brackets in the equation, we get:

$$-\,i\,\hbar\,\Big(n\,\Psi[n+1] - n\,\Psi[n] - n\,\Psi[n+1] - \Psi[n+1] + n\,\Psi[n]\Big) = i\,\hbar\,\Psi[n] \tag{8}$$

This equation gives the equality:

$$\Psi[n+1] = \Psi[n] \quad (for\ all\ n \in \mathbb{Z}) \tag{9}$$

which means $\Psi[n] = \text{const}$, i.e., $\Psi[n] = \Psi[0]$ for all $n \in \mathbb{Z}$. Similar relations can be obtained for other type of standard finite differences.

As a result, we prove that the canonical commutation relation for discrete quantum mechanics, which is based on the standard finite differences, holds only for the degenerate case of a constant wave function. This fact does not allow us to build a sensible discrete quantum mechanics based on the standard finite differences.

Remark 1. It is well-known that the finite difference of integer order n cannot be considered as an exact discretization of the derivative of order n [13,14]. For example, the forward finite difference ${}^{f}\Delta^{1}_{h}$

of first order with step h can be formally represented [13] by using the Taylor series with respect to h in the form:

$$ {}^{f}\Delta_h^1 = h\frac{d}{dx} + \frac{h^2}{2}\frac{d^2}{dx^2} + \frac{h^3}{6}\frac{d^3}{dx^3} + ... = \exp\left(h\frac{d}{dx}\right) - I \tag{10} $$

where $\exp\left(h\frac{d}{dx}\right)$ is the shift operator. Therefore, the finite differences of order $n \in \mathbb{N}$ give only approximation of the derivatives of integer orders d^n/dx^n. The expression ${}^{f}\Delta_h^n/h^n$ gives the derivative d^n/dx^n at $h \to 0$ only. Using formal inverting of Equation (10), we get the equation:

$$ h\frac{d}{dx} = \log\left(1 + {}^{f}\Delta_h^1\right) = \sum_{j=0}^{\infty} \frac{(-1)^j}{j+1}\, {}^{f}\Delta_h^{j+1} \tag{11} $$

which holds in the sense that left and right sides of Equation (11) give the same result when applied to polynomials and analytic functions. Equations (10) and (11) allow us to see that the standard finite differences of the first order cannot be considered as an exact discrete analog of the derivatives of first order (see also [9]). As a result, these differences cannot give an exact discretization of the momentum operator in the coordinate representation of the quantum mechanics.

Remark 2. It is well-known that the standard Leibniz rule is not satisfied for the standard finite differences [13,14]. If we use the forward difference Equation (4) or other type of standard finite differences, then the standard Leibniz rule is violated,

$$ {}^{f}\Delta^1 \left(\Psi_1[n]\,\Psi_2[n]\right) \neq \left({}^{f}\Delta^1\,\Psi_1[n]\right)\Psi_2[n]) + \Psi_1[n]\left({}^{f}\Delta^1\,\Psi_2[n]\right) \tag{12} $$

As a result, the main characteristic algebraic property of the derivative of first order is not satisfied. For standard finite differences, the product rule has the form:

$$ {}^{f}\Delta^1 \left(\Psi_1[n]\,\Psi_2[n]\right) = \left({}^{f}\Delta^1\,\Psi_1[n]\right)\Psi_2[n]) + \Psi_1[n]\left({}^{f}\Delta^1\,\Psi_2[n]\right) + \left({}^{f}\Delta^1\,\Psi_1[n]\right)\left({}^{f}\Delta^1\,\Psi_2[n]\right) \tag{13} $$

This violation of the standard Leibniz rule leads us to the inequality:

$$ \hat{p}(n\Psi[n]) \neq \hat{p}(n)\,\Psi[n] - n\,\hat{p}(\Psi[n]) \tag{14} $$

for the representations of the momentum operator $\hat{p}$ by the standard finite differences (see Equation (3)). As a result, we get a violation of the canonical commutation relations for these representations.

Remark 3. Let us note that Equation (3) with Equation (4) cannot be considered as a correct discrete analog of the momentum operator Equation (2). The difference operator, which is defined by Equation (4), does not have p as its classical limit, and therefore cannot be used to quantize the momentum. Therefore, we cannot use the discretization of the momentum in the form of Equation (3). As a result, we have an additional argument, which allows us to state that the standard discretization of derivatives of integer orders cannot be a correct exact discrete representation of the quantum theory. At the same time, the standard discretization of the Schrödinger equation is based on the replacement $\hat{p}^2/2\mu = -(\hbar^2/2\mu)d^2/dx^2$ by the standard difference operators such as $-(\hbar^2/2\mu)\,{}^{c}\Delta^2$, where ${}^{c}\Delta^2$ is the central finite difference of second order. Note that this representation is usually interpreted as a nearest-neighbor interaction, and it is used in quantum mechanics.

Remark 4. To save the commutation relations of discrete quantum mechanics, we can use non-standard finite difference schemes for differential operators. For example, the exact discretization of differential equations of integer orders has been considered in [15–17] and [18–20]. It has been proved that, for differential equations, there are "locally exact" finite-difference discretization, where the local truncation errors are zero. A main disadvantage of this discretization of the integer-order derivatives is that these differences strongly depend on the form of the considered differential equation and the parameters of these equations. In addition, the suggested differences do not have the same algebraic properties as derivative operators of integer orders (for details see [10]). As a result, this approach does not satisfy the "discrete-continuous" correspondence principle [10] according to which the correspondence between the "continuous" and "discrete" quantum theories lies not so much in the limiting agreement when the step of discretization tends to zero as in the fact that mathematical operations on the two theories obey, in many cases, the same laws. As a result, we have that the standard and previously proposed non-standard discretizations of derivatives of integer orders cannot give an exact discrete representation of the quantum theory that satisfies the "discrete-continuous" correspondence principle.

3. Exact Discretization of Quantum Mechanics

In papers [6,7,9–12], a new mathematical tool was proposed, which is based on differences that are represented by infinite series. The suggested approach allows us to build sensible discrete quantum mechanics, since the proposed differences are exact discrete analogs of derivatives. [7,9–12].

The mathematical basis of the suggested exact discretization is the following correspondence principle: the correspondence between the discrete theory and the continuous theory lies not so much in the limiting condition when the steps of discretization tend to zero as in the fact that mathematical operations on these theories should obey the same algebraic laws in many cases.

In some sense, the proposed exact discretization is similar to quantization and the suggested principle is similar to the Dirac's correspondence principle: "The correspondence between the quantum and classical theories lies not so much in the limiting agreement when $h \to 0$ as in the fact that mathematical operations on the two theories obey in many cases the same laws" (see page 649 of [21]).

The proposed difference operators, which are the exact discretization of differential operators of integer or non-integer orders, satisfy the same characteristic algebraic relations as the differential operators. In addition, the suggested differences operators allow us to have difference equations, whose solutions are equal to the solutions of corresponding differential equations.

Note that the standard finite differences cannot be considered as an exact discretization of derivatives since these differences violate the Leibniz rule and the expression of derivatives of entire functions [10].

In the coordinate representation, the coordinate and momentum operators are defined by the equations:

$$\hat{q}\,\Psi[n] = n\,\Psi[n] \tag{15}$$

$$\hat{p}\,\Psi[n] = -\,i\,\hbar\,{}^{\mathcal{T}}\boldsymbol{\Delta}^1\,\Psi[n] \tag{16}$$

where ${}^{\mathcal{T}}\boldsymbol{\Delta}^1$ is the $\mathcal{T}$-difference of first order,

$${}^{\mathcal{T}}\boldsymbol{\Delta}^1\,\Psi[n] := \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \frac{(-1)^m}{m}\,\Psi[n-m] \tag{17}$$

In general, in Equation (17) summation means the Poisson–Abel summation [10]. The Hamiltonian can be defined by the equation:

$$\hat{H} = -\frac{\hbar^2}{2\,\mu}\,{}^{\mathcal{T}}\boldsymbol{\Delta}^2 + U[n] \tag{18}$$

where μ is the mass, ${}^{\mathcal{T}}\mathbf{\Delta}^2$ is the $\mathcal{T}$-difference of second order [9,10] that is defined by the equation:

$$ {}^{\mathcal{T}}\mathbf{\Delta}^2\, \Psi[n] := - \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \frac{2\,(-1)^m}{m^2}\, \Psi[n-m] - \frac{\pi^2}{3} \Psi[n] \tag{19} $$

The time-independent Schrödinger equation $\hat{H}\,\Psi[n] = \Psi[n]\,E$ has the form of the following $\mathcal{T}$-difference equation:

$$ - \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \frac{2\,(-1)^m}{m^2}\, \Psi[n-m] + \left(\frac{2\,\mu}{\hbar^2}\,(E - U[n]) - \frac{\pi^2}{3} \right) \Psi[n] = 0 \tag{20} $$

This equation is the eigenvalue equation for an infinite matrix [22]. The time-independent Schrödinger equation is an eigenvalue problem for infinite matrices [23–25]. The solutions of Equation (20) are considered in [9,10].

4. Exact Discrete Analog of Canonical Commutation Relation

Using Equations (15) and (16), the canonical commutation relation of the suggested discrete quantum mechanics,

$$ \hat{q}\,\hat{p}\,\Psi[n] - \hat{p}\,\hat{q}\Psi[n] = i\,\hbar\,\Psi[n] \tag{21} $$

is represented by the $\mathcal{T}$-difference equation:

$$ -\,i\,\hbar\, \Big(n\, {}^{\mathcal{T}}\mathbf{\Delta}^1\, \Psi[n] - {}^{\mathcal{T}}\mathbf{\Delta}^1\, (n\,\Psi[n]) \Big) = i\,\hbar\,\Psi[n] \tag{22} $$

where we assume that $\Psi[m]$ satisfies the condition:

$$ \sum_{m=-\infty}^{+\infty} (-1)^m\, \Psi[m] = 0 \tag{23} $$

To prove the canonical commutation relation Equation (22), we consider an action of the $\mathcal{T}$-difference Equation (17) on the product n and $\Psi[n]$. Using Equation (17), we have:

$$ {}^{\mathcal{T}}\mathbf{\Delta}^1\, (n\,\Psi[n]) = \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \frac{(-1)^m}{m}\, (n-m)\,\Psi[n-m] \tag{24} $$

Applying the properties of the discrete convolution, Equation (24) is rewritten in the form:

$$ {}^{\mathcal{T}}\mathbf{\Delta}^1\, (n\,\Psi[n]) = \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} \frac{(-1)^{n-m}}{n-m}\, m\,\Psi[m] \tag{25} $$

Using the equality:

$$ \frac{m}{n-m} = \frac{n}{n-m} - 1 $$

we get:

$$
\begin{aligned}
l^{\mathcal{T}}\boldsymbol{\Delta}^1\,(n\,\Psi[n]) &= n\sum_{\substack{m=-\infty\\ m\neq n}}^{+\infty}\frac{(-1)^{n-m}}{n-m}\,\Psi[m]-\sum_{\substack{m=-\infty\\ m\neq n}}^{+\infty}(-1)^{n-m}\,\Psi[m]\\
&= n\,{}^{\mathcal{T}}\boldsymbol{\Delta}^1\,\Psi[n]-(-1)^n\sum_{\substack{m=-\infty\\ m\neq n}}^{+\infty}(-1)^m\,\Psi[m]\\
&= n\,{}^{\mathcal{T}}\boldsymbol{\Delta}^1\,\Psi[n]-(-1)^n\sum_{m=-\infty}^{+\infty}(-1)^m\,\Psi[m]+\Psi[n]
\end{aligned}
\tag{26}
$$

Using the assumption given by Equation (23), the second term of Equation (26) is equal to zero. As a result, we obtain Equation (26) in the form:

$$
{}^{\mathcal{T}}\boldsymbol{\Delta}^1\,(n\,\Psi[n]) = n\,{}^{\mathcal{T}}\boldsymbol{\Delta}^1\,\Psi[n]+\Psi[n] \tag{27}
$$

Substitution of Equation (27) into Equation (22) gives an equality that proves the canonical commutation relation Equation (21).

Note that generalization of commutation relations for non-Hamiltonian and dissipative quantum systems is considered in Chapter 19 of [2].

Remark 5. The Stone–von Neumann theorem shows that representations of the canonical commutation relations by self-adjoint operators are unique, up to unitary transformations. Therefore, we can assume that there exists a unitary transformation from the discrete representation, which is suggested in this paper, to the standard "continuous" representation of the canonical commutation relations. We suggested the exact discretization of the standard quantum mechanics and the canonical commutation relations. This discretization is exact in the sense that the following correspondence principle holds "The correspondence between the 'continuous' and 'discrete' quantum theories lies not so much in the limiting agreement when the step of discretization tends to zero as in the fact that mathematical operations on the two theories obey in many cases the same laws". In addition, the suggested difference operators can be used not only in the canonical commutation relations, but also in the Schrödinger equations [11]. The suggested $\mathcal{T}$-differences do not depend on the parameters and form of equations.

Remark 6. In discrete quantum mechanics, we can assume that the discrete wave-functions $\Psi[n]$ belong to the Hilbert space l^2 of square-summable sequences. In general, we can use the sequence space l^p ($p > 0$), which is the linear space consisting of all discrete functions (sequences) $\Psi[n]$, where $n \in \mathbb{Z}$, satisfying the inequality:

$$
\sum_{n=-\infty}^{+\infty}|\Psi[n]|^p < \infty \tag{28}
$$

If $p \geq 1$, then we can define a norm on the l^p-space by the equation:

$$
\|\Psi\|_p := \left(\sum_{n=-\infty}^{+\infty}|\Psi[n]|^p\right)^{1/p} \tag{29}
$$

The sequence space l^p with $p > 0$, is a complete metric space with respect to this norm, and therefore it is a Banach space. We can assume that $\Psi[n]$ belongs to the Hilbert space l^2 of square-summable sequences to apply the Fourier series transform. It is known that if $1 \leq p < q$, then $l^q \subset l^p$. Therefore, $l^q \subset l^2$ if $q > 2$, and we will consider $\Psi[m] \in l^q$ with $q \geq 2$.

Theorem. *The $\mathcal{T}$-differences ${}^{\mathcal{T}}\boldsymbol{\Delta}^n\,\Psi[m] := \sum_{k=-\infty}^{\infty} K_n(k)\,\Psi[m-k]$, which are defined by convolutions of its kernels $K_n(m) \in l^p$ $(p > 1)$ and $\Psi[m] \in l^q$ $(q \geq 2)$, are operators $l^q \to l^r$ that map the discrete function $\Psi[m] \in l^q$ $(q \geq 2)$ into functions $g[m] \in l^r$ $(r \geq 2)$ such that:*

$$g[m] := {}^{\mathcal{T}}\boldsymbol{\Delta}^n\,\Psi[m] \in l^r \tag{30}$$

where $m \in \mathbb{Z}$, and,

$$\frac{1}{r} + 1 = \frac{1}{p} + \frac{1}{q} \tag{31}$$

Proof. It is known that if $\Psi[m] \in l^q$ and $K_n[m] \in l^p$, then the inequality:

$$\|K_n * \Psi\|_r \leq \|K_n\|_p\, \|\Psi\|_q \tag{32}$$

holds, where r is defined by Equation (31) and the star $*$ denotes the convolution. Inequality Equation (32) is the Young's inequality for convolutions (see [26,27] and Theorem 276 of [28]). Using the Young's inequality in the form:

$$\|\,{}^{\mathcal{T}}\boldsymbol{\Delta}^n\,\Psi[m]\|_r = \|K_n\, *\, \Psi\|_r \leq \|K_n\|_p\, \|\Psi\|_q \tag{33}$$

we get:

$$g[m] := {}^{\mathcal{T}}\boldsymbol{\Delta}^n\Psi[m] \in l^r \tag{34}$$

if the condition given by Equation (31) holds, and $\Psi[m] \in l^q$ $(q \geq 2)$ and $K_n(m) \in l^p$ $(p > 1)$.

Using the Theorem, it is easy to see that the result of the action of operators ${}^{\mathcal{T}}\boldsymbol{\Delta}^{2n}$ on the function $\Psi[n] \in l^2$ also belongs to the Hilbert space l^2 of square-summable sequences, i.e.,

$${}^{\mathcal{T}}\boldsymbol{\Delta}^{2n}\,\Psi[m] \in l^2 \tag{35}$$

since condition Equation (31) holds. As a result, the $\mathcal{T}$-differences are the operators on the Hilbert space l^2 of square-summable sequences, i.e., ${}^{\mathcal{T}}\boldsymbol{\Delta}^{2n}: \quad l^2 \to l^2$.

5. Expectation Value and Normalization Condition

Expectation value can be defined by using the inner product of the Hilbert space l^2 of square-summable sequences. In this approach, we have the expectation value:

$$\langle \hat{A} \rangle_D := \sum_{n=-\infty}^{+\infty} \Psi^*[n]\, \hat{A}\, \Psi[n] \tag{36}$$

where function $\Psi[n]$ belongs to the Hilbert space l^2. In this case, the normalization condition has the form $\|\Psi\|_2 = 1$.

There is a possibility to define the expectation value by a somewhat different method. In papers [9,10], a difference of negative integer order $n = -1$ has been suggested in the form:

$${}^{\mathcal{T}}\boldsymbol{\Delta}^{-1}\Psi[n] := \sum_{\substack{m=-\infty \\ m \neq 0}}^{+\infty} \pi^{-1}\, Si(\pi\, m)\, \Psi[n-m] \tag{37}$$

where $Si(z)$ is the sine integral. Note that this difference is the inverse to the first-order $\mathcal{T}$-difference given by Equation (17), i.e.,

$${}^{\mathcal{T}}\boldsymbol{\Delta}^{1}\, {}^{\mathcal{T}}\boldsymbol{\Delta}^{-1}\Psi[n] = \Psi[n] \tag{38}$$

and we have the equality for the second-order $\mathcal{T}$-difference (19) in the form

$$ {}^{\mathcal{T}}\mathbf{\Delta}^{2}\, {}^{\mathcal{T}}\mathbf{\Delta}^{-1}\Psi[n] = {}^{\mathcal{T}}\mathbf{\Delta}^{1}\Psi[n] \tag{39}$$

Difference Equation (37) can be considered as an exact discretization of the antiderivative. This allows us to define exact discrete analogs of the expectation value and normalization condition.

For one-dimensional cases, the standard normalization condition has the form

$$\int_{-\infty}^{+\infty} |\Psi(x)|^2 \, dx = 1 \tag{40}$$

The improper integral is the limit of the definite integral,

$$\lim_{a\to\infty} \int_{-a}^{+a} |\Psi(x)|^2 \, dx = 1 \tag{41}$$

Equation (41) can be represented in the form:

$$\lim_{a\to\infty} \Big(F_{|\Psi|^2}(a) - F_{|\Psi|^2}(-a) \Big) = 1 \tag{42}$$

where $F_{|\Psi|^2}(x)$ is the antiderivative of the function $|\Psi(x)|^2$. Using $\mathcal{T}$-difference of order $n = -1$, which is an exact discrete analog of antiderivative, we can write the corresponding normalization condition of discrete quantum mechanics in the form:

$$\lim_{n\to\infty} \Big(({}^{\mathcal{T}}\mathbf{\Delta}^{-1}|\Psi|^2)[n] - ({}^{\mathcal{T}}\mathbf{\Delta}^{-1}|\Psi|^2)[-n] \Big) = 1 \tag{43}$$

Substitution of Equation (37) into Equation (43) gives:

$$\lim_{n\to\infty} \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \pi^{-1}\, Si(\pi\, m)\ \Big(|\Psi[n-m]|^2 - |\Psi[-n-m]|^2 \Big) = 1 \tag{44}$$

This equation gives an exact form of the normalization condition for the discrete wave function.

Using the definition of the sine integral, we can see that Equation (44) in some sense is analogous to a representation of Equation (41) using the Whittaker–Shannon interpolation formula or the Whittaker cardinal series [29].

Similarly, we can define the expectation value for the discrete quantum mechanics. In the standard case, the expectation value of a quantum observable $\hat{A}$ of a systems with a pure state $\Psi(x)$ is defined as:

$$\langle \hat{A} \rangle := \int_{-\infty}^{+\infty} \Psi^*(x)\, (\hat{A}\Psi)(x)\, dx \tag{45}$$

Let us denote the expectation value of the discrete quantum mechanics by the symbol $\langle\ \rangle_D$. Using the difference given by Equation (37), the exact discrete analog of Equation (45) has the form:

$$\langle \hat{A} \rangle_D := \lim_{n\to\infty} \Big({}^{\mathcal{T}}\mathbf{\Delta}^{-1}\Psi^*[n]\, (\hat{A}\Psi)[n] - {}^{\mathcal{T}}\mathbf{\Delta}^{-1}\Psi^*[-n]\, (\hat{A}\Psi)[-n] \Big) \tag{46}$$

Substitution of Equation (37) into Equation (46) gives the exact expression:

$$\langle \hat{A} \rangle_D := \lim_{n\to\infty} \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \pi^{-1}\, Si(\pi\, m)\ \big(\Psi^*[n-m]\, (\hat{A}\Psi)[n-m] - \Psi^*[-n-m]\, (\hat{A}\Psi)[-n-m] \big) \tag{47}$$

This is the definition of the expectation value of quantum observable $\hat{A}$ of the suggested exact discretization of quantum mechanics.

Remark 7. Using the fact that the discrete analogue of the antiderivative Equation (37) is the inverse operation to taking the $\mathcal{T}$-difference of the first order, and the fact that this $\mathcal{T}$-difference satisfies the standard Leibniz rule, it is easy to show that the proposed exact discretization of the momentum operator defines a self-adjoint discrete operator.

6. Uncertainty Relation of Discrete Quantum Mechanics

The uncertainty relation states a fundamental limit on the standard deviations of incompatible quantum observables, such as position $\hat{q}$ and momentum $\hat{p}$. The uncertainty relation is a basic inequality of quantum mechanics. It was introduced by Heisenberg [30] for the coordinate $\hat{q}$ and momentum $\hat{p}$ in the form of an approximate relation $\Delta\hat{q}\Delta\hat{p} \sim \hbar$. The uncertainty relation in the form of the inequality:

$$\Delta\hat{q}\, \Delta\hat{p} \geq \frac{\hbar}{2} \tag{48}$$

was proved by Kennard [31], where $\Delta\hat{q}$ and $\Delta\hat{p}$ are the standard deviations of the coordinate $\hat{q}$ and momentum $\hat{p}$, which are defined by $\Delta\hat{A} = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$. The inequality Equation (48) has been extended by Robertson [32] for two arbitrary quantum observables. A stronger inequality has been suggested by Schrödinger [33] and Robertson [34] in the form:

$$(\Delta\hat{A})^2\, (\Delta\hat{B})^2 \geq \frac{1}{4}\Big(\langle \hat{A}\hat{B} - \hat{B}\hat{A} \rangle^2 + \langle \hat{A}\hat{B} + \hat{B} \rangle^2\Big) \tag{49}$$

where $\hat{A}$ and $\hat{B}$ are an arbitrary pair of quantum observables. Different generalizations of the Heisenberg and Schrödinger–Robertson uncertainty relations have been considered by several authors [35–39] in the case of pure and of mixed states of Hamiltonian systems. The uncertainty relations for open quantum systems are considered by Sandulescu and Scutaru [40,41] for an example of quantum harmonic oscillator with linear friction. Note that general properties of uncertainty relations for non-Hamiltonian quantum systems are described in [42].

Let us consider the uncertainty relation for discrete quantum observables $\hat{q}$ and $\hat{p}$ that are defined by Equations (15) and (16). The derivation of this relation is analogous to the standard (non-discrete) case [42]. We use the notation :

$$\hat{A} = \hat{q} - \langle \hat{q} \rangle_D\, I, \quad \hat{B} = \hat{p} - \langle \hat{p} \rangle_D\, I \tag{50}$$

where I is an identity operator. The operators $\hat{q}$ and $\hat{p}$ are self-adjoint operators ($\hat{A}^\dagger = \hat{A}$, $\hat{B}^\dagger = \hat{B}$).

Let us consider the operator $\hat{C} = \lambda\hat{A} + i\hat{B}$, where λ is a complex number. Using the non-negativity property of expectation values in the form $\langle \hat{C}^\dagger \hat{C} \rangle_D \geq 0$, we get the inequality:

$$\langle (\lambda^* \hat{A} - i\hat{B})(\lambda\hat{A} + i\hat{B}) \rangle_D \geq 0$$

for all $\lambda \in \mathbb{C}$. Using the linear property for the expectation values, we obtain:

$$\lambda^* \lambda \left\langle \hat{A}^2 \right\rangle_D + i\lambda^* \langle \hat{A}\hat{B} \rangle_D - i\lambda \langle \hat{B}\hat{A} \rangle_D + \left\langle \hat{B}^2 \right\rangle_D \geq 0 \tag{51}$$

Inequality Equation (51) can be rewritten in the form:

$$(\lambda_1^2 + \lambda_2^2) \left\langle \hat{A}^2 \right\rangle_D - \hbar\lambda_1 \langle \hat{A} * \hat{B} \rangle_D + 2\lambda_2 \langle \hat{A} \circ \hat{B} \rangle_D + \left\langle \hat{B}^2 \right\rangle_D \geq 0$$

where we use the notations:

$$\hat{A} * \hat{B} := \frac{1}{i\hbar}(\hat{A}\hat{B} - \hat{B}\hat{A}), \quad \hat{A} \circ \hat{B} := \frac{1}{2}(\hat{A}\hat{B} + \hat{B}\hat{A}) \tag{52}$$

and λ_1 and λ_2 are real and imagine parts of $\lambda = \lambda_1 + i\lambda_2$. Using Euler's formula, we represent λ_1 and λ_2 in the form $\lambda_1 = x\cos\varphi$, $\lambda_2 = x\sin\varphi$. Then,

$$\left\langle \hat{A}^2 \right\rangle_D x^2 + \left(2\left\langle \hat{A}\circ\hat{B}\right\rangle_D \sin\varphi - \hbar\left\langle \hat{A}*\hat{B}\right\rangle_D \cos\varphi\right) x + \left\langle \hat{B}^2 \right\rangle_D \geq 0 \tag{53}$$

This inequality should be satisfied for all $\varphi \in \mathbb{R}$ and all $x \geq 0$. The inequality $ax^2 + bx + x \geq 0$ holds for all $x \geq 0$ for two cases: (I) the discriminant $D = b^2 - 4ac$ is negative; (II) the conditions $D \geq 0$, $b \geq 0$, $c \geq 0$ hold. Using the phase shift method for linear combination of sine and cosine of equal angles, it is easy to prove that the condition:

$$b = 2\left\langle \hat{A}\circ\hat{B}\right\rangle_D \sin\varphi - \hbar\left\langle \hat{A}*\hat{B}\right\rangle_D \cos\varphi \geq 0$$

cannot be realized for all $\varphi \in \mathbb{R}$. Therefore, the discriminant of the quadratic polynomial Equation (53) should be negative:

$$D = \left(2\left\langle \hat{A}\circ\hat{B}\right\rangle_D \sin\varphi - \hbar\left\langle \hat{A}*\hat{B}\right\rangle_D \cos\varphi\right)^2 - 4\left\langle \hat{A}^2 \right\rangle_D \left\langle \hat{B}^2 \right\rangle_D \leq 0 \tag{54}$$

for all $\varphi \in \mathbb{R}$. We can write Equation (54) as the inequality:

$$\left\langle \hat{A}^2 \right\rangle_D \left\langle \hat{B}^2 \right\rangle_D \geq \frac{1}{4}\left(2\left\langle \hat{A}\circ\hat{B}\right\rangle_D \sin\varphi - \hbar\left\langle \hat{A}*\hat{B}\right\rangle_D \cos\varphi\right)^2 \tag{55}$$

that should satisfied for all $\varphi \in \mathbb{R}$. Using the relation of the phase shift method, we get,

$$\left\langle \hat{A}^2 \right\rangle_D \left\langle \hat{B}^2 \right\rangle_D \geq \left(\frac{\hbar^2}{4}\left\langle \hat{A}*\hat{B}\right\rangle_D^2 + \left\langle \hat{A}\circ\hat{B}\right\rangle_D^2\right)\sin^2(\varphi - \alpha) \tag{56}$$

where

$$\sin\alpha = \frac{\hbar\left\langle \hat{A}*\hat{B}\right\rangle_D}{\sqrt{\hbar^2\left\langle \hat{A}*\hat{B}\right\rangle_D^2 + 4\left\langle \hat{A}\circ\hat{B}\right\rangle_D^2}}$$

Using the inequality $\sin^2(\varphi+\alpha) \leq 1$, we obtain the uncertainty relation:

$$\left\langle \hat{A}^2 \right\rangle_D \left\langle \hat{B}^2 \right\rangle_D \geq \frac{\hbar^2}{4}\left\langle \hat{A}*\hat{B}\right\rangle_D^2 + \left\langle \hat{A}\circ\hat{B}\right\rangle_D^2 \tag{57}$$

Substitution of Equation (50) into Equation (57) gives:

$$(\Delta\hat{q})^2 (\Delta\hat{p})^2 \geq \frac{\hbar^2}{4}\langle \hat{q}*\hat{p}\rangle_D^2 + \left(\langle \hat{q}\circ\hat{p}\rangle_D - \langle \hat{q}\rangle_D \langle \hat{p}\rangle_D\right)^2 \tag{58}$$

This is the uncertainty relation of the Schrödinger-Robertson-type, where the quantum observables of position $\hat{q}$ and momentum $\hat{p}$ are defined by Equations (15) and (16) and the expectation values is represented by Equation (46) or (47).

The standard form of the Heisenberg uncertainty relation:

$$\left\langle (\hat{q} - \langle \hat{q}\rangle_D I)^2 \right\rangle_D \left\langle (\hat{p} - \langle \hat{p}\rangle_D I)^2 \right\rangle_D \geq \frac{\hbar^2}{4} \tag{59}$$

is realized only if we use the commutation relation in the form of Equation (22) and the condition:

$$\langle \hat{q}\hat{p} + \hat{p}\hat{q}\rangle_D - 2\langle \hat{q}\rangle_D \langle \hat{p}\rangle_D = 0 \tag{60}$$

The condition $\langle \hat{q}\hat{p} + \hat{p}\hat{q} \rangle_D = 0$, which is considered in [38], cannot give Heisenberg's uncertainty relation [42], since the expectation values $\langle \hat{q} \rangle_D$ and $\langle \hat{p} \rangle_D$ can be nonzero. In this case ($\langle \hat{q}\hat{p} + \hat{p}\hat{q} \rangle_D = 0$), we should use the inequality:

$$\left\langle (\hat{q} - \langle \hat{q} \rangle_D I)^2 \right\rangle_D \left\langle (\hat{p} - \langle \hat{p} \rangle_D I)^2 \right\rangle_D \geq \frac{\hbar^2}{4} \langle \hat{q} * \hat{p} \rangle_D^2 + \langle \hat{q} \rangle_D^2 \langle \hat{p} \rangle_D^2 \tag{61}$$

Using the notation given by Equation (52) and commutation relation Equation (22) for inequality Equation (58), we obtain:

$$\left\langle (\hat{q} - \langle \hat{q} \rangle_D I)^2 \right\rangle_D \left\langle (\hat{p} - \langle \hat{p} \rangle_D I)^2 \right\rangle_D \geq \frac{\hbar^2}{4} + \frac{1}{4} \Big(\langle \hat{q}\hat{p} + \hat{p}\hat{q} \rangle_D - 2 \langle \hat{q} \rangle_D \langle \hat{p} \rangle_D \Big)^2 \tag{62}$$

for coordinate and momentum of Hamiltonian system.

In the general case, condition Equation (60) is not satisfied and we should use an uncertainty relation in the form of Equation (62) instead of relation Equation (59).

7. Conclusions

In this paper, we use the recently proposed exact discretization approach [9–12] and the corresponding lattice calculus [6,7], which are based on $\mathcal{T}$-differences of integer and non-integer orders. Using this tool, we demonstrate that there is a possibility to build sensible and consistent discrete quantum mechanics by the suggested $\mathcal{T}$-differences of integer orders. In this paper, we proved that the proposed discrete ($\mathcal{T}$-difference) analog of the canonical commutation and uncertainty relations hold exactly.

We assume that the proposed approach based on suggested $\mathcal{T}$-differences can have a wide range of applications since its allows us to take into account the main characteristic algebraic properties of the differential operators. These difference operators are exact discretization of differential operators because $\mathcal{T}$-differences satisfy the same algebraic characteristic relations as derivatives. In addition, the $\mathcal{T}$-difference equations have solutions that are equal to the solutions of corresponding differential equations.

Let us list some of the closest possible applications of the proposed approach that are based on the proposed $\mathcal{T}$-differences: (1) the lattice models with long-range interactions [7], which can be described by the suggested differences; (2) the lattice regularization of quantum field theories [8]; (3) the computer simulations of nonlinear Schrödinger equations (see Section 7 of [11]); (4) the discrete analogs of the methods of the quantum mechanics; and (5) the development of modern methods of the difference calculus [14] for the $\mathcal{T}$-difference equations.

The proposed $\mathcal{T}$-difference approach can be generalized to theory when deformed commutation relations are used instead of the usual ones. In this generalization, it must take into account that the $\mathcal{T}$-differences are used for exact discrete analogs of quantum observables in the coordinate representation.

In this paper, we consider only Hamiltonian quantum systems with pure quantum states that are described by wave functions. The suggested approach to exact discretization of quantum theory can be applied for non-Hamiltonian and open quantum systems, where quantum states are represented by density operator and dynamics are described by quantum Markovian or non-Markovian master equations [2]. For example, the stationary states of non-Hamiltonian, dissipative and open quantum systems [43,44] can be described in the framework of the discrete quantum theory as a generalization of pure stationary states described in [11].

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