Iranian Journal of Numerical Analysis and Optimization
Vol. ??, No. ??, ??, pp ??
https://doi.org/??
https://ijnao.um.ac.ir/

Research Article

Quantum solutions of a nonlinear Schrödinger equation

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Abstract

In the present paper, we precisely conduct a quantum calculus method for the numerical solutions of PDEs. A nonlinear Schrödinger equation is considered. Instead of the known classical discretization methods based on the finite difference scheme, Adomian method, and third modified versions, we consider a discretization scheme leading to subdomains according

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Received ??? ; revised ??? ; accepted ???

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How to cite this article
Arfaoui, S. and Ben Mabrouk, A., Quantum solutions of a nonlinear Schrödinger equation. *Iran. J. Numer. Anal. Optim.*, ??; ??(??): ??-??. ??

to q-calculus and provide an approximate solution due to a specific value of the parameter q. Error estimates show that q-calculus may produce efficient numerical solutions for PDEs. The q-discretization leads effectively to higher orders of convergence provided with faster algorithms. The numerical tests are applied to both propagation and interaction of soliton-type solutions.

AMS subject classifications (2020): Primary 35C08, 35Q55; Secondary 65L80, 81Q05.

Keywords: NLS equation; Quantum calculus; Numerical solution; Error estimates.

1 Introduction

The present paper is devoted essentially to the development of a numerical scheme to approximate the solution of a Nonlinear Schrödinger (NLS) equation in a quantum calculus framework. The aim crosses in fact the restriction to the resolution of such an equation and goes further to show that q-calculus may provide a good framework for numerical solutions of PDEs in general. It is well known that a major literature on the numerical solutions of PDEs is based on classical methods, such as finite difference, finite elements and volumes, Fourier analysis, and recently wavelets. See [7, 5, 9, 10, 11, 12, 16, 19, 28].

The NLS equation is strongly linked to the modeling of real physical phenomena, such as Newton's laws and energy conservation in classical mechanics, the behavior of dynamical systems, the description of a particle in a nonrelativistic setting in quantum mechanics, and so on.Therefore, the NLS equation attracted researchers from both theoretical and applied mathematics and physics. See [16, 19, 22, 28].

Originally, Schrödinger's stated a linear form describing a moving particle according to the model equation

$$\Delta\psi + \frac{8\pi^2 m}{\hbar^2}\,(E - V(x))\,\psi = 0, \tag{1}$$

where ψ is known as a wave function, m is the particle mass, $\hbar$ is the Planck's constant, E is the energy, and V is a potential (see [13, 20, 23, 25, 29]).

Based upon the analogy between mechanics and optics, Schrödinger applied a perturbation method to show an equivalence between his wave function in mechanics and Heisenberg's matrix. This gave rise next to the time dependent model

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi - \gamma|\psi|^2\psi \quad \text{in } \mathbb{R}^N, \tag{2}$$

known as the cubic NLS equation. Next, different variants and forms have been developed and investigated by researchers in different fields (see [1, 4, 17, 24, 26]).

The present paper is devoted to the development of a numerical method based on q-calculus to approximate the solution of a reduced NLS equation in $\mathbb{R}$ written on the form

$$\begin{cases} iu_t + \Delta u + f(u) = 0, & (x,t) \in \Omega \times (t_0, +\infty), \\ u(x,t_0) = u_0(x), & x \in \Omega, \\ \dfrac{\partial u}{\partial n}(x,t) = 0, & (x,t) \in \partial\Omega \times (t_0, +\infty). \end{cases} \tag{3}$$

We consider a domain Ω in $\mathbb{R}$, and t_0 is a real parameter fixed as the initial time, u_t is the first order partial derivative in time, Δ is the Laplace operator, and $\dfrac{\partial}{\partial n}$ is the outward normal derivative. Moreover, $\partial\Omega$ is the boundary of Ω. Also, $u = u(x,t)$ and $u_0 = u_0(x)$ are complex valued functions. In addition, f is a nonlinear function of u assumed to be at least continuous.

In [15], the stationary solutions of problem (3) have been studied using direct methods issued from the equation on the whole space. See also [14]. In [6], a Lyapunov–Sylvester method has been applied to solve numerical NLS and Heat equations.

The organization of the present work will be as follows. In section 2, the q-calculus essential tools will be reviewed. Section 3 is devoted to the presentation of our main method. The discrete quantum version of a cubic NLS equation will be developed with the necessary analysis of convergence, stability, solvability, and consistency. Section 4 is the subject of numerical experimentation due to our theoretical part. We conclude afterward.

2 Quantum calculus toolkit

One of the interesting fields of extensions of real analysis is the so-called q-theory, which provides some discrete and/or some refinement of continuous analysis in subspaces such as $\mathbb{R}_q$, which is composed of the discrete grid $\pm q^n$, $n \in \mathbb{Z}$, $q \in (0,1)$. Recall that for all $x \in \mathbb{R}^*$, there exists a unique $n \in \mathbb{Z}$ such that $q^{n+1} < |x| \leq q^n$, which guarantees some density of the set $\mathbb{R}_q$ in $\mathbb{R}$.

This section aims to introduce some basic concepts of q-theory. We present some definitions, notations, and properties of q-derivatives, which will be useful later. Backgrounds on q-theory may be found in [3, 21] and the references therein.

For $0 < q < 1$, denote

$$\mathbb{R}_q = \{\pm q^n, \ \ n \in \mathbb{Z}\} \ \text{ and } \ \widetilde{\mathbb{R}}_q^+ = \mathbb{R}_q^+ \bigcup \{0\}.$$

We propose in this section to recall two basic functions that are applied almost everywhere in q-theory and its applications. See, for example, [18].

Definition 1. The q-derivative of a function is defined by

$$D_q f(x) = \begin{cases} \dfrac{f(x) - f(qx)}{(1-q)x}, & x \neq 0, \\ f'(0)\ , & else, \end{cases}$$

provided that f is differentiable at 0.

The operator D_q is the q-analogue of the classical derivative, as indeed, if f is differentiable, we get

$$\lim_{q \longrightarrow 1} D_q f(x) = \frac{df(x)}{dx}.$$

Many concepts of derivatives and integration rules have been extended for the case of q-calculus.

The only drawback of the q-calculus is the fact that they remain applied and investigated especially in harmonic functional analysis for the major part of the literature. A first step ahead has been conducted by Koornwinder and Swarttouw when studying Jackson's third q-Bessel function. Their work motivates researchers to develop different q-differential operators. Recently,

q-calculus returns to take place in PDEs. Indeed, consider, for example, an elliptic equation

$$\Delta u + f(u, x) = 0, \tag{4}$$

where f is a suitable function, generally nonlinear in u. We may search for a numerical q-approximation by considering a grid points in $\mathbb{R}_q$ instead of finite difference/finite elements used usually. In q-theory, we already have a q-analog of the Laplace operator expressed as

$$\Delta_q u(x) = \frac{qu(q^{-1}x) - (1+q)u(x) + u(qx)}{x^2}.$$

For $x = q^n$ in $\mathbb{R}_q^+$, we get from (4),

$$u_{n+1} - (1+q)u_n + qu_{n-1} = -(1-q)^2 q q^{2n} f_n,$$

where $u_n = u(q^n)$ and f_n is some discretization of $f(u, x)$. We thus obtain a recursive equation permitting to compute u_n recursively. More about applications of q-calculus in partial differential equations may be found in [3]. A widely known example in q-theory is the Bessel type equation

$$\begin{cases} \Delta_q u(x) = -\lambda^2\, u(x), \\ u(0) = 1,\ u'(0) = 0, \end{cases}$$

($\lambda \in \mathbb{C}$), which has as unique solution a modified q-Bessel function. In the present paper, we will exploit the q-calculus to develop numerical solutions of some PDEs.

3 The discrete NLS equation

In this section, we develop the details of our numerical method. For this aim, we fix $\Omega = [0, 1]$ and $t_0 = 0$. Fix also a time step $l_k = (1-q)q^k$, and for $k \in \mathbb{N}$, we denote t_k the kth instant. For $n \in \mathbb{N}$, we denote $x_n = q^n$, and $h_n = (1-q)q^n$ the nonuniform space step. Denote also $u_n^k = u(t_k, x_n)$ the net function and U_n^k its numerical approximation (the solution of the discrete problem). We discretize problem (3) as follows,

$$i\frac{U_n^{k+1}-U_n^k}{l_k}+\frac{2q}{1+q}\frac{qU_{n-1}^k-(1+q)U_n^k+U_{n+1}^k}{h_n^2}+f(U_n^k)=0. \qquad (5)$$

By setting for $n,k\in\mathbb{N}$,

$$\delta_n^k=\frac{2q}{1+q}\frac{l_k}{h_n^2}, \qquad \text{and} \qquad \sigma_n^k=\frac{2q}{1+q}\frac{l_k}{h_n^2}i=\delta_n^k i,$$

the discrete problem (5) becomes

$$U_n^{k+1}=q\sigma_n^kU_{n-1}^k+(1-(1+q)\sigma_n^k)U_n^k+\sigma_n^kU_{n+1}^k+F_n^k, \qquad (6)$$

where $F_n^k=il_kf(U_n^k)$. Now, denote for $k\in\mathbb{N}$,

$$U^k=(U_n^k)_{n\in\mathbb{N}},$$

the infinite vector of the numerical solution at the time k. Denote also

$$\beta_n^k=1-(1+q)\sigma_n^k.$$

We get the following dynamical infinite matrix-vector system:

$$U^{k+1}=A_kU^k+F^k, \qquad (7)$$

where A_k is the infinite tridiagonal matrix with elements

$$A_k=\begin{pmatrix}
1-\sigma_0^k & \sigma_0^k & 0 & \dots & \dots & \dots & \dots & \dots & \dots \\
q\sigma_1^k & \beta_1^k & \sigma_1^k & 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & q\sigma_2^k & \beta_2^k & \sigma_2^k & 0 & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & q\sigma_3^k & \beta_3^k & \sigma_3^k & 0 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & q\sigma_n^k & \beta_n^k & \sigma_n^k & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots
\end{pmatrix}.$$

Infinite (especially tridiagonal) matrices are met in many fields and have been applied widely. Finite forms are met in PDEs, such as finite difference methods, in numerical analysis. See, for instance, [2, 8]. In mathematics, infinite tridiagonal matrices are initially related to the so-called Jacobi operators (see [27]).

Note in problem (7) that a main difference with classical methods, such as the finite difference method, is the possibility to relax one assumption on boundary conditions. We only need such an assumption for one extremity of the domain Ω.

Now, observe that, for each k, we get

$$|1-\sigma_0^k|^2 = 1+|\delta_0^k|^2 > |\delta_0^k|^2 = |\sigma_0^k|^2,$$

and similarly,

$$|\beta_n^k|^2 = 1+(1+q)^2|\delta_n^k|^2 > (1+q)^2|\delta_n^k|^2 = (1+q)^2|\sigma_n^k|^2,$$

which means that the matrix A_k is a dominant-diagonal matrix, which guarantees the solvability of our discrete scheme and leads to the following theorem.

Theorem 1. The numerical problem (7) is uniquely solvable, for $k \geq 2n+1$.

In terms of the classical numerical schemes, such as the finite difference, the assumption $k > n$ replaces the assumption $l = o(h^2)$, where l and h are the time and space steps for the finite difference scheme.

To investigate the stability of the numerical scheme, we propose to apply the Lyapunov criterion for stability, which states that a dynamical system $\mathcal{L}(U_k, U_{k-1}, \dots) = 0$ is stable in the Lyapunov sense if, for any bounded initial solution U_0, the solution U_n remains bounded for all $n \geq 0$ uniformly on n. Here, we will precisely prove the following result.

Lemma 1. The solution U^k is bounded independently of k whenever the initial solution U^0 is bounded.

Proof. We will proceed by recurrence on k. Assume firstly that $\|U^0\| \leq \eta$, for some η positive. It follows from the assumption $k \geq 2n+1$ that

$$|\sigma_n^k| \leq \frac{2q}{(1+q)(1-q)}.$$

Therefore, using system (6), for $k = 0$, we obtain

$$U_n^1 = q\sigma_n^0 U_{n-1}^0 + (1-(1+q)\sigma_n^0)U_n^0 + \sigma_n^0 U_{n+1}^0 + F_n^0.$$

As U^0 is bounded, and the nonlinear function f is continuous, we deduce that U^1 is bounded. So, assume that U^k is bounded independently of k. Using system (6), we get

$$|U_n^{k+1}| \leq \frac{1+3q}{1-q}|U_n^k| + |F_n^k|.$$

Using the recurrence hypothesis and again the continuity of the nonlinear function F, we deduce that

$$|U_n^{k+1}| \leq \frac{2(1+q)}{1-q}C,$$

where $C > 0$ is a constant independent of k.

The consistency of the proposed method is evaluated by means of the local truncation error arising from the discretization scheme. Assuming that the solution u is sufficiently regular, we get the principal part as

$$\mathcal{L}(u)(x,t) = \frac{il_k}{2}u_{tt} + \frac{(1-q)h_n}{3q}u_{xxx} + o(l_k + h_n). \tag{8}$$

It is clearly observable that the truncation operator $\mathcal{L}(u)$ goes to 0 as n, k go to ∞. This yields that the quantum numerical scheme is consistent at a minimum order 1 in time and space.

To finish with the convergence of the numerical method, we apply the Lax–Richtmyer equivalence criterion, which states that for consistent numerical approximations, stability and convergence are equivalent. We thus obtain the following lemma. □

Lemma 2. As the numerical scheme is consistent and stable, it is then convergent.

Indeed, recall here that we have already proved in (8) that the used scheme is consistent. Next, Lemma 1 yields the stability of the scheme. Consequently, the Lax equivalence theorem guarantees the convergence.

4 Numerical implementations

We propose in this experimental part to develop numerical examples to validate the theoretical results developed in the previous sections. We will use an L_2 discrete norm to evaluate the error between the exact solutions and

the numerical ones as

$$\|X\|_2 = \Big(\sum_i |X_i|^2\Big)^{1/2},$$

for any vector (series) $X = (X_i)$ eventually in $L^2(\mathbb{C})$. Denote u^k the net function $u(x, t^k)$ and U^k the numerical solution. We propose to compute the discrete error

$$\text{Er} = \max_k \|U^k - u^k\|_2 \tag{9}$$

on the grid (x_n), $n \geq 0$.

We take for the rest $f(u) = |u|^2 u$, which gives the original cubic NLS equation. We next take the classical soliton-type solution

$$u(x,t) = \sqrt{\frac{2a}{q_s}} \exp\Big(i\big(\frac{1}{2}cx - \theta t + \varphi\big)\Big) sech\Big(\sqrt{a}(x - ct) + \phi\Big),$$

where a, q_s, c, $\theta = \dfrac{c^2}{4} - a$, φ and ϕ are some appropriate constants. For t fixed, this function decays exponentially as $|x| \to \infty$. It is a soliton-type disturbance, which travels with speed c and with a-governed amplitude. See [5, 6, 10, 11, 12, 20, 22, 28, 29].

4.1 Propagation of a single soliton

In the first experimentation, we focus on a single-soliton-type particle. The computations are done for $0 \leq x \leq 1$ and $0 \leq t \leq 1$. We fix the q parameter to many different values according to the closeness to 0 or to 1. So, let $q \in \{q_i = \frac{i}{8},\ i = 1, \ldots, 7\}$. We also fix the soliton parameters $a = 0.01$, $q_s = 1$, $c = 0.1$, and the phase parameters $\varphi = \phi = 0$. Figures 1 and 2 illustrate two cases of the numerical solution for the propagation of a single soliton issued from our quantum numerical scheme.

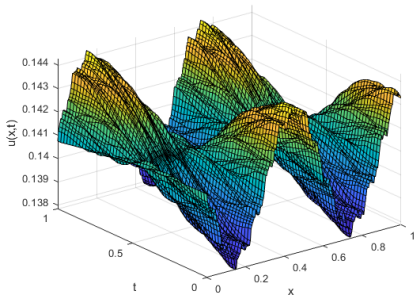

Figure 1: Propagation of a single soliton, for $q = \frac{1}{8}$.

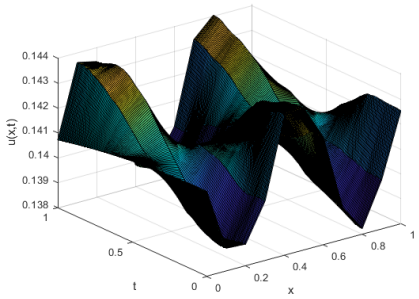

Figure 2: Propagation of a single soliton, for $q = \frac{3}{8}$.

Tables 1 and 2 illustrate the error estimates between the numerical solution and the exact one for different values of the quantum parameter q, and for different values of the maximal time index K. The space grid is fixed to N number of points. Truncating in an order N for practice feasibility of the system (7), we denote TrU_N^k the truncated vector

$$TrU_N^k = [U_0^k, U_1^k, \ldots, U_N^k]^T,$$

and TrF_N^k the truncated vector

$$TrF_N^k = [F_0^k, F_1^k, \ldots, F_N^k]^T,$$

where the upper script ^{T} is for the transpose. We denote similarly, TrA_k^N the truncated matrix

$$TrA_k^N = \begin{pmatrix} 1-\sigma_0^k & \sigma_0^k & 0 & \dots & \dots & \dots \\ q\sigma_1^k & \beta_1^k & \sigma_1^k & 0 & \ddots & \ddots \\ 0 & q\sigma_2^k & \beta_2^k & \sigma_2^k & 0 & \ddots \\ 0 & 0 & q\sigma_3^k & \beta_3^k & \sigma_3^k & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & q\sigma_N^k & \beta_N^k \end{pmatrix}.$$

The system (7) will be approximated by

$$TrU_N^{k+1} = TrA_k^N TrU_N^k + TrF_N^k.$$

Table 1: Error estimates for a single soliton for $N = 20$

				$K = 10$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$1.17\,10^{-5}$	$1.28\,10^{-5}$	$2.41\,10^{-4}$	$2.52\,10^{-4}$	$2.18\,10^{-4}$	$3.11\,10^{-4}$	$2.87\,10^{-4}$
				$K = 15$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$2.01\,10^{-6}$	$2.32\,10^{-6}$	$3.01\,10^{-5}$	$2.84\,10^{-5}$	$2.71\,10^{-5}$	$3.01\,10^{-5}$	$2.77\,10^{-5}$
				$K = 20$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$1.27\,10^{-7}$	$1.44\,10^{-7}$	$1.23\,10^{-6}$	$2.15\,10^{-6}$	$2.53\,10^{-6}$	$2.01\,10^{-5}$	$2.76\,10^{-5}$

Table 2: Error estimates for a single soliton for $N = 50$

				$K = 10$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$1.17e-5$	$1.28e-5$	$2.41e-4$	$2.52e-4$	$2.18e-4$	$3.11e-4$	$2.87e-4$
				$K = 15$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$2.01e-6$	$2.32e-6$	$3.01e-5$	$2.84e-5$	$2.71e-5$	$3.01e-5$	$2.77e-5$
				$K = 20$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$1.27e-7$	$1.44e-7$	$1.23e-6$	$2.15e-6$	$2.53e-6$	$2.01e-5$	$2.76e-5$

It is notable from Tables 1 and 2 that the numerical quantum discrete scheme converges with good error estimates. This encourages to application such a discretization idea for solving more complicated problems.

4.2 Interaction of two solitons

We consider here two solitons traveling with the same speed but in opposite directions in order to obtain the interaction phenomenon. The computations are done as in the previous experimentation on the space domain $\Omega_x = [0, 1]$ and a time space also $I_t = [0, 1]$. We fix the q parameter as previously to $q \in \{q_i = \frac{i}{8},\ i = 1, \ldots, 7\}$. We also fix the soliton parameters as follows:

- For the first soliton, we put $a = 1$, $q_s = 2$, $c = 4$, $\varphi = 0$, and $\phi = 15$.
- For the second soliton, we put $a = 2,25$, $q_s = 2$, $c = -4$, $\varphi = 0$, and $\phi = -7,5$.

As in the previous experimentation, Tables 3 and 4 illustrate the error estimates between the numerical solution and the exact one for different values of the quantum parameter q, and for different values of the maximal time index K. The space grid is fixed to a number N of points.

Table 3: Error estimates for two-interacted solitons for $N = 20$

$K = 10$							
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$2.27e-5$	$2.45e-5$	$2.51e-4$	$2.76e-4$	$3.14e-4$	$3.44e-4$	$4.02e-4$
$K = 15$							
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$2.11e-6$	$2.18e-6$	$2.05e-5$	$2.61e-5$	$2.85e-5$	$3.12e-5$	$4.05e-5$
$K = 20$							
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$1.92e-7$	$2.02e-7$	$2.15e-6$	$2.44e-6$	$3.21e-6$	$3.32e-5$	$3.876e-5$

Table 4: Error estimates for two-interacted solitons for $N = 50$

				$K = 10$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$125e-5$	$1.34e-5$	$1.44e-4$	$2.21e-4$	$2.43e-4$	$2.31e-4$	$2.15e-4$
				$K = 15$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$1.15e-6$	$1.27e-6$	$1.32e-5$	$1.17e-5$	$1.95e-5$	$2.02e-5$	$2.33e-5$
				$K = 20$			
q	q_1	q_2	q_3	q_4	q_5	q_6	q_7
Er	$1.16e-7$	$1.31e-7$	$2.13e-6$	$2.23e-6$	$2.27e-6$	$2.47e-5$	$2.55e-5$

As in the previous case, we notice from Tables 3 and 4 that the numerical quantum discretization yielded a very close approximated solution to the exact one. This is clearly shown by the error estimates, where the maximum error is estimated by 10^{-4} over all the values of the quantum parameter q in two Tables 3 and 4. This finding motivates the use of a quantum numerical scheme for more general and/or complicated PDEs.

Remark 1. We know that in the case of classical finite difference and finite element methods, the error is generally estimated in the power of the space step $h = \Delta x$, which in turn is related to the size N of the mesh or, equivalently, the number of the discretization points. In these cases, we obtain an error to the order h^α or equivalently, the order $N^{-\alpha}$, for some exponent α. In the new q-quantum case, we obtain an error to the order of $q^{\alpha N}$, which has the form of a geometric sequence with a ratio q^α in the interval $(0, 1)$, which therefore converges to 0 more rapidly than the previous sequence $N^{-\alpha}$. We then gain a quick and more precise scheme. These facts make it unnecessary to concretely develop the numerical comparisons, as we know in advance that the classical schemes will give higher error, lower speed of convergence, and higher running time. Mathematically, it is easy to see that for $\alpha, \beta > 0$, it holds that for all $\varepsilon > 0$, there exisits $N_0 \in \mathbb{N}$, such that $q^{\beta N} N^\alpha \leq \varepsilon$, for all $N \geq N_0$. This means that, the q-quantum scheme, even at a lower order $\beta < \alpha$ is better than the classical schemes. In other words, the q-quantum scheme does not necessitate calibrating the discretization to get higher orders for convergence, consistency, and good stability, as it is done for the

classical finite difference and finite element methods with implicit method, Crank–Nicolson, centering/decentering method, higher regularity order finite elements bases, and so on.

5 Conclusion

In the present paper, the principal aim was to test the efficiency of the quantum calculus in the approximation of the solutions of PDEs. As a prototypical example, we applied q-calculus to derive a numerical scheme for the well-known cubic NLS equation. As expected, the q-calculus yielded good approximations illustrated by low error estimates. The findings in the present paper make therefore good motivation to continue to exploit quantum calculus for the numerical (and also exact) solutions of different types of PDEs. Comparisons with other models, such as finite difference, finite volumes, and also wavelets as recent developments in mathematical analysis are fascinating and motivating future extensions. Compared to the classical finite difference scheme method, we may conclude theoretically that, in fact, the present quantum scheme is more efficient, as it is based on geometric sequences of time and space steps, which surely converge more rapidly than arithmetic discretizations. Therefore, we expect that involving or including hybrid schemes may induce the best results. Finally, an interesting question raised from the present work may be formulated as follows: Given an infinite matrix that is truncated in an order n. We know that at most in $\mathbb{C}$, any truncation has at most n eigenvalues. What can we expect for the original linear operator defined by means of the infinite matrix? This gives rise to possible chaotic behavior as a future study of the present case of matrices, which are issued from parabolic, hyperbolic PDEs.

Acknowledgment

The authors would like to thank the editor of IJNAO and the anonymous reviewers for their insightful comments and suggestions which helped to improve our work.

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