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A NEW APPROACH TO NUMERICAL SOLUTION OF THE NONSTATIONARY SCHRÖDINGER EQUATION WITH POLYNOMIAL NONLINEARITY

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In the present paper we propose a new technique for the numerical solution of the Schrödinger equation with the enough common type nonlinearity

$$i\psi_t + \psi_{xx} + f(|\psi|^2)\psi = 0, \tag{1}$$

where in the term of f we imply the polynomial of the l-th degree:

$$f \equiv f(|\psi|^2) = \sum_{l=0}^{N} \alpha_l |\psi|^{2l} = \alpha_0 + \alpha_1|\psi|^2 + \alpha_2|\psi|^4 + \cdots + \alpha_N|\psi|^{2N}. \tag{2}$$

Depending on the number of the series members and also on the coefficients of (2) (we suppose that $\alpha_0, \alpha_1, \cdots$ are, in general, arbitrary), eq.(1) arises in various branches of physics. For example, in the case of $N = 0$ and $\alpha_0 = U \equiv U(x)$, eq.(1) describes the motion of quantum particles (electrons, protons and so on) in the external field U (1926, E. Schrödinger). The eq.(1) for $N = 1$ is the Schrödinger equation with the cubic nonlinearity (the so called $\psi^3 - NLSE$). Corresponding to the sign of $\alpha_1 = const$ ($\alpha_0 = 0$), the $\psi^3 - NLSE$ has a wide application in physics. For $\alpha_1 > 0$, it describes the nonideal Bose gas of the attracting particles [1], the propagation of light beams in a nonlinear dispersive media [2] (the propagation of "bright solitons"), and it also arises in the study of some problems of the theory of magnetism and molecular crystals. The $\psi^3 - NLSE$ with the $\alpha_1 = const < 0$ serves as a phenomenogical model of superfluidity for the inhomogeneous and nonstationary order parameter ψ [3], it describes the propagation of "dark solitons" in nonlinear optics [4], the nonideal Bose gas of the repulsive particles[5] etc.

The addition of the following members in (2), apart from the pure mathematical variety, leads to the description of the more complicated phenomena. For $N = 2$ one has the $\psi^3 - \psi^5 - NLSE$, which were applied to the nuclear hydrodynamics with Skyrma forces[6], to the Bose gas with two- particle attractive and three- particle repulsive δ- function-like interaction potential [7] and so on. In view of such a rich application in physics and other sciences, the development of the numerical methods for solving the NLSE is still a challenging task. A good library of the various finite difference, spectral, iterative and other numerical methods can be found in the remarkable work of Taha and Ablowitz [8]. Recently [9], a modification of the multigrid methods for the parallel numerical simulation of the $\psi^3 - NLSE$ was proposed.

Nevertheless, many methods applied to numerical analysis of the NLSE, will works when the initial condition or some information about the initial configuration is known. In the case of the absence of such an information we propose the following scheme to solve the NLSE. Using the idea of "continuation on parameter" [10], we introduce a parametric dependence on T for $f(|\psi|^2)$ the following way:

$$f(T) = Tf(|\psi|^2), \tag{3}$$

Further, by carrying out the discretization of (1), taking into account the (3), we will have:

$$i\frac{\psi_m^{n+1} - \psi_m^n}{\Delta t} + \frac{(\delta^2\psi)_m^n + (\delta^2\psi)_m^{n+1}}{2(\Delta x)^2} + T\frac{\Phi(\psi_m^n) + \Phi(\psi_m^{n+1})}{2} = 0. \tag{4}$$

Here in (4) we introduce the following notation for the space differences and nonlinear term approximation:

$$(\delta^2\psi)_m^n = \psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n, \quad \Phi(\psi_m^n) = f(|\psi_m^n|^2)\psi_m^n, \qquad (5).$$

It should be noted that the first order time differencing in (4), as well as the approximations introduced in (5) are not unique and we imply, of course, the existence of the other approximations here. The main idea of the developed scheme is that the numerical solution of the all $\psi^{2l+1} - NLSE$ can be carried out on the basis of the solution of the linear problem. Starting from the same initial condition at $T = 0$, we will, depending on the type of nonlinearity in (1), come to the various results at $T = 1$. Thus, the solution of $\psi_m^n = \psi(m\Delta x, n\Delta t) \equiv \psi(x,t)$ will be a function of T for every value of the parameter $T \in [0,1]$. Obviously, for $T = 1$ we have the original system of equations (1)-(2), and for $T = 0$ we obtain a more simple linear problem. We introduce a discretization on T : $T_j; j = 0,1,\cdots,M(T_0 = 0, T_M = 1)$. In order to find a solution of the problem (1)-(2) in the point T_{j+1}, having the $\psi_m^n(T_j)$, one can use Newton's method. We suppose that the difference $|T_{j+1} - T_j|$ is enough small and we have the good initial approximation for Newton's method:

$$F'(\vec{p}, z_k)v_k = -F(\vec{p}, z_k),$$

$$\vec{p} = \{T, \psi_m^n, \alpha_0, \alpha_1, \cdots\}, \quad z_k = \{\psi_m^{n+1,k}\},$$

and

$$z_{k+1} = z_k + v_k, \quad k = 0,1,\cdots.$$

It is important that the proposed approach can easily be generalized for investigation of multidimensional nonlinear Schrödinger systems. The more detailed practical analysis of the described above numerical scheme is in progress. The some realization of the similar method has been done in [11], to carry out the numerical analysis of three- dimensional polaron equations.

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О новом подходе к численному анализу нестационарного уравнения Шредингера с полиномиальной нелинейностью

В данной работе изложен новый подход к численному анализу нестационарного уравнения Шредингера с полиномиальной нелинейностью. Используя идею «продолжения по параметру» для уравнения Шредингера:

$$i\psi_t + \psi_{xx} + Tf(|\psi|^2)\psi = 0,$$

где $f(|\psi|^2)$ — полином l-й степени, вводится параметрическая зависимость от T. Основная идея предложенной схемы заключается в том, что численное решение всех ψ^{2l+1} — НУШ может быть проведено на основе единой линейной задачи. Стартуя с одного и того же начального условия при $T = 0$, мы приходим, в зависимости от типа нелинейности, к различным результатам при $T = 1$.

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A New Approach to Numerical Solution of the Nonstationary Schrödinger Equation with Polynomial Nonlinearity

In the present paper we propose a new technique for the numerical solution of the Schrödinger equation with the polynomial nonlinearity. Using the idea of «continuation on parameter», we introduce a parametric dependence of T for $f(|\psi|^2)$, where $f(|\psi|^2)$ is the polynomial of the l-th degree of the nonstationary Schrödinger equation:

$$i\psi_t + \psi_{xx} + Tf(|\psi|^2)\psi = 0.$$

The main idea of the developed scheme is that the numerical solution of the all ψ^{2l+1} — NLSE can be carried out on the basis of the solution of the linear problem. Starting from the same initial condition at $T = 0$, we will, depending on the type of nonlinearity, come to the various results at $T = 1$.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

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