Numerical Investigation of a Class of Nonlinear Schrödinger Equations

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ABSTRACT

This paper numerically investigates the space-localized spherically symmetric, stationary, and singularity-free solutions of the Nonlinear Schrödinger equation when the nonlinearity is a step function. Previously no-node solutions have been obtained analytically. Here, it is shown that localized stationary solutions with one node and two nodes also exist.

I. INTRODUCTION

The Schrödinger equation is

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + U(x) \psi \quad (1)$$

where $\hbar$ is Planck's constant, m is the mass of the particle, $U(x)$ is the potential in which the particle moves, and $\psi = \psi(x, t)$ is the wave-function for that particle [1].

This is the fundamental equation of non-relativistic quantum mechanics. It describes the motion of electrons and other elementary particles. It is a linear partial differential equation.

In contemporary physics nonlinear versions of Schrödinger equation are studied. Their form is

$$i \frac{\partial \psi}{\partial t} = -\mu \nabla^2 \psi + \psi G(\psi^* \psi) \quad (2)$$

where $\mu > 0$ is a real constant and G is a real function of $|\psi|^2 = \psi^* \psi$.

The space-localized solutions of the nonlinear Schrödinger equations are interpreted as representations of elementary particles. Only three nonlinear Schrödinger equations are known to be solvable analytically: the one with a logarithmic nonlinearity, the one with $G(\psi^* \psi) = k \psi^* \psi$ (k is a constant), and G is a step function [1-4].

In the case when G is a step function, only no-node space-localized solutions were obtained analytically. Using numerical calculations I have found one-node and two-node space-localized solutions. This is evidence that space-localized solutions of any number of nodes exist when the nonlinearity is a step function.

The goal of this paper is to numerically investigate the space localized, spherically symmetric, stationary, and singularity-free solutions of the NLS (Nonlinear Schrödinger Equation) when G is a step function.

II. THE EQUATION FOR SPHERICALLY SYMMETRIC STATIONARY SOLUTIONS

We start with equation (2). Then we use that fact that stationary solutions are of the form

$$\psi = \varphi e^{-i\omega t} \quad (3)$$

where $\varphi = \varphi(x)$ is a function of the coordinates $x = (x_1, x_2, x_3)$ only. By substituting equation (3) into equation (2) the NLS becomes

$$\omega \varphi = -\mu \nabla^2 \varphi + \varphi G(\varphi^* \varphi) \quad (4)$$

Now we can rewrite equation (4) as the following

$$\mu \nabla^2 \varphi = (G - \omega) \varphi \quad (5)$$

Figure 1. Three types of solution to the non-linear Schrodinger equation (NLS) for three values of the shooting parameter, v_0 .

Since we are looking for spherically symmetric solutions the following must be true for ϕ

$$\nabla^2 \phi = \frac{1}{r} \frac{d^2(r\phi)}{dr^2} \quad (6)$$

where $\phi = \phi(r)$ is expressed as a function of r .

Using this we find that our NLS becomes

$$\frac{\mu}{r} \frac{d^2(r\phi)}{dr^2} = (G - \omega)\phi \quad (7)$$

which is an ordinary differential equation (ODE). For our convenience we will define a new variable,

$$u = r\phi \quad (8)$$

Now our ODE can be written as

$$\mu \frac{d^2 u}{dr^2} = (G - \omega)u \quad (9)$$

Next, we define $G = G\left(\frac{|u|}{r}\right)$ to be the step

function:

$$G = \begin{cases} \omega_0 & \frac{|u|}{r} < 1 \\ 0 & \frac{|u|}{r} \geq 1 \end{cases} \quad (10)$$

The shooting method and Runge-Kutta method can now be used to find solutions to the following set of equations:

$$\begin{cases} \frac{du}{dr} = v \\ \frac{dv}{dr} = (G - \omega)u \end{cases} \quad (11)$$

with initial conditions

$$u_0 = 0 \quad (12)$$

and $v_0 =$ shooting parameter.

III. THE SHOOTING METHOD

Before the Runge-Kutta method can be applied to the NLS equation, equation (9) must be reduced to a system of two first order ordinary differential equations

$$\frac{du}{dr} = v \quad (14)$$

$$\frac{dv}{dr} = \left(\frac{G}{\omega_0} - \omega \right) u \quad (15)$$

Since the NLS equation is of order 2, two initial conditions must be specified in order to determine a particular solution to the equations. These initial conditions are u_0 and v_0 . Because we are looking for singularity-free solutions, $|u| \rightarrow 0$ as $r \rightarrow 0$ (because

$\varphi = \frac{u}{r}$ must remain finite). From this we get

that $u_0 = 0$. Now we have to determine the “shooting parameter” v_0 . Since we are looking for space-localized solutions we know that $|u| \rightarrow 0$ as $r \rightarrow \infty$. Thus, we can just vary the parameter v_0 until a space-localized solution is found. v_0 describes the initial slope of the particular solution, and thus by varying this parameter we may “shoot” for the solution we desire (a space-localized solution). Figure 1 shows an example of three solutions obtained with three different values of the parameter v_0 .

Now the Runge-Kutta method may be used to find solutions to the NLS equation.

IV. RESULTS

First we have to verify that the shooting method works. To do this we compare the analytical result for the no-node solution with the results of the numerical method for the no-node solution. The analytical solution is

$$\varphi = \frac{r_1}{\sqrt{\omega r}} \sin(\sqrt{\omega r}) \quad \text{for } 0 \leq r \leq r_1 \quad (16a)$$

$$\varphi = \frac{r_1}{r} e^{\sqrt{1-\omega}(r_1-r)} \quad \text{for } r_1 \leq r \leq \infty \quad (16b)$$

where r_1 is the value of r at which the step occurs. See Georgieva and Bodurov [3] for more details on the analytical solution. Figure 2 illustrates a comparison between the numerical and analytical solutions.

a. One-Node Solution:

We have varied the parameter ω , so as to include values throughout its entire domain. The shooting method was then used to determine the value v_0 for which the one-node solution exists. Figures 3, 4, and 5 represent some of these solutions for $\omega = 0.1$, 0.5, and 0.9, respectively.

b. Two-Node Solutions:

Once again we have varied the parameter ω , so as to include values throughout its entire domain. The shooting method was then used to determine the value v_0 for which the two-node solution exists. Figures 6, 7, and 8 represent some of these solutions for $\omega = 0.1$, 0.5, and 0.9, respectively.

V. L_2 -NORM

Now that we have demonstrated the existence of stationary solutions with multiple nodes, we can calculate the L_2 -norm N of

$\varphi = \frac{u}{r}$ for the one-node and two-node solutions by numerical integration. The integration is performed by applying the trapezoidal rule to u^2 at different values of ω .

By the definition of the L_2 -norm we have

$$N = \int_{R^3} \varphi^2 dx dy dz \quad (17)$$

where $\mathcal{R}^3$ stands for all space and $dx dy dz$ stands for the volume element. In our case, we have

$$N = \int_{R^3} \varphi^2 dx dy dz = \int_0^\infty \left(\frac{u}{r} \right)^2 4\pi r^2 dr = 4\pi \int_0^\infty u^2 dr \quad (18)$$

since $\varphi = \frac{u}{r}$ and $dx dy dz = 4\pi r^2 dr$ because of spherical symmetry.

a. No-Node

Once again we will verify that the numerical procedure works, through comparison with the analytical solution. Figures 9 and 10 show that the L_2 -norm has a single minimum

at $\omega \approx 0.931$, which agrees with the results of the analytical solution.

b. One-Node

Now that we have validated the numerical procedure, we shall apply it to the one-node solutions. The results are shown in Figures 11 and 12.

Figure 2. (Top left) Verification of the Shooting Method: A comparison between the analytical solution (solid line) and the numerical solution (dotted line) for $\omega = 0.5$ and $v_0 = 3.332074$. The two solutions overlay each other quite closely.

Figure 3. (Middle left) An example of a One-Node solution, with $\omega = 0.1$ and $v_0 = 18.331585$.

Figure 4. (Bottom left) An example of a One-Node solution, with $\omega = 0.5$ and $v_0 = 7.088522$.

Figure 5. (Top right)
An example of a One-Node solution, with $\omega = 0.9$ and $v_0 = 4.277392$.

Figure 6. (Middle right)
A Two-Node solution, with $\omega = 0.1$ and $v_0 = 27.653563$.

Figure 7. (Bottom right)
A Two-Node solution, with $\omega = 0.5$ and $v_0 = 10.778026$.

Figure 8. (Top left) A Two-Node solution, with $\omega = 0.9$ and $v_0 = 6.562161$.

Figure 9 (Middle left) and **Figure 10** (Bottom left) show that the L_z -norm has a single minimum in the No-Node case at $\omega \approx 0.931$, which agrees with the results of the analytical solution.

Figures 11 and 12 show that the L_2 -norm has a single minimum.

c. Two-Node

Now we shall apply the procedure to the two-node solutions. The results are shown in Figures 13 and 14.

Figure 11 (Top right) and **Figure 12** (Middle right) show that the L_2 -norm also has a single minimum in the case of the One-Node solutions.

Figure 13 (Bottom right) and **Figure 14** (Top next page) show that the L_2 -norm also has a single minimum in the case of the Two-Node solutions.

Figure 14 (at left) shows that the L_2 -norm also has a single minimum in the case of the Two-Node solutions.

CONCLUSION

The above results are presented as evidence that space-localized solutions of one node and two nodes exist, when the non-linearity in the NLS is a step function. Based on the results of this paper, we can conjecture that solutions with any number of nodes exist. We have also demonstrated that the no-node, one-node, and two-node solutions all have a single minimum for their L_2 -norm.

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