ON THE CONVERGENCE OF THE SOLUTION OF SCHRODINGER EQUATION FOR FINITE DIFFERENCE METHOD

D. Kobaidze[1,a], T. Gagnidze [1], T. Tchelidze [1], T. Davitashvili [1], H. Meladze [2]

[1]*Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia,* [a]*daviti.kobaidze708@ens.tsu.edu.ge*
[2]*Muskhelishvili Institute of Computational Mathematics*

Abstract. In the present paper we investigate the convergence of solution of the Schrodinger equation for potential energy of particular conditions. The issue is crucial for application of numerical techniques, such as finite difference method.

Keywords: Schrodinger equation, Finite difference method

1. Introduction

Quantum mechanical processes and dynamics of quantum particles are described by Schrodinger equation [1]. It is well known, that Schrodinger equation has exact, analytical solutions (wave functions and energy spectrum),only in few cases. There are a lot of interesting from practical and theoretical point of view potentials, for which it is unable to write down exact solutions. Therefore, it is of great importance to proceed numerical calculations. One of the most important and practically usable way to solve the equation is the finite difference method [2]. The problem is that when we solve the equation numerically, firstly it must be known if the solution is convergent. One of our main purpose is to show that the solution of Schrodinger type equation converges when we use finite difference method to solve it.

2. Theoretical framework

Let's discuss the following equation:

$$L(u) = u''(x) - p(x)u(x) = -f(x), \qquad x \in [0, X]; \tag{1}$$

$$u(0) = a, \quad u(X) = b\,. \tag{2}$$

On $[0, X]$ segment, let's define regular grid with the step $h = \frac{X}{N}$. Denote this grid by $\overline{\omega_h}$. On this grid we change the equation (1) by the finite difference equation, which reads as follows:

$$l(y_n) = \frac{y_{n+1} - 2y_n + y_{n-1}}{h^2} - p_n y_n = -f_n\,, \quad n = 1,2,3, \dots, N-1 \tag{3}$$

In this case boundary conditions will be:

$$y_0 = a, \quad y_N = b\,. \tag{4}$$

It can be proven, that if $p(x) \geq 0$, than problems (3), (4) have unique solution which converges.

We also estimate the expected error of the method, which turns out to be satisfactory.

Acknowledgment:
The work is supported by Shota Rustaveli National Science Foundation of Georgia, Grant Number STEM-22-188.

References:

[1] David J. Griffiths, Introduntion to Quantum Mechanics, Prentice Hall, 1995
[2] Randall J. LeVeque, Finite Difference Methods for Differential Equations, 2004