Journal of the Nigerian Association of Mathematical Physics
Volume 7(2003)

Analysis of the nonlinear Schrödinger Equation in an infinite potential well

A. N. Njah
Department of Physics, University of Agriculture, Abeokuta, Nigeria.
(e-mail: njahabdul@yahoo.com)
and
R. Akin-Ojo
Department of Physics, University of Ibadan, Ibadan, Nigeria.

Abstract

The Nonlinear Schrödinger Equation (NLSE) *in units of* $\hbar = 1$

$$i\frac{\partial \psi}{\partial t} + \alpha \frac{\partial^2 \psi}{\partial x^2} + \beta |\psi|^p \psi = 0; \ \psi = u(x)e^{-i\lambda t}$$

where α *and* β *are real parameters, p is a positive integer and* λ *is the eigenvalue (energy) is solved by numerical and perturbation methods in an infinite potential well vis-`a-vis the linear Schrödinger* (LSE). *The eigenvalue* λ_n *for the* n^{th} *eigenvalue in the well is found for the cases* $p = 2[4]$ *to be given by* $\lambda_n = an^2 + bn + c$, *where* a = 2.46831[2.46773], b = -0.065982[-0.039568] and c = 1[1] using the *numerical method. Using the perturbation method leads to similar results. These results are comparable with those of the* LSE: $\lambda_n = kn^2$, *where* k = 2.5. α *and* β *have the effect of increasing the values of the* λ's. *Also as p increases* λ_n *for the* NLSE *tends to* λ_n *for the* LSE. *The analysis confirms that the* NLSE *describes small amplitude waves, which are also self energizing.*

pp 39 - 46

1.0 Introduction

The Nonlinear Schrödinger Equation

$$i\psi_t + \psi_{xx} \pm |\psi|^2 \psi = 0 \tag{1.1}$$

have diverse applications. For that reason an analysis of the NLSE vis-`a-vis the LSE is necessary. This paper tackles the numerical and pertubative solution of the NLSE in an infinite potential well.

The most important applications of the NLSE's are to some phenomena of nonlinear optics. The NLSE with (+) sign describe the self-focussing of the carrier wave which leads to the envelope-solution. The equation with (-) sign describes the self-defocussing which leads to the dark-solution. Other important applications are to packets of water waves and plasma waves [1]. It also has a geometric application in the context of the three-dimensional motion of a vortex [2]. Most physical phenomena are, however, described by the perturbed NLSE

$$i\psi_t + \psi_{xx} \pm |\psi|^2 \psi = \varepsilon R(\psi) \tag{1.2}$$

where the perturbation $\varepsilon R(\psi)$ takes various forms depending on the physical system in question [3]. If the perturbation comes from some potential $V\psi$ then equation (1.2) gives a generalization of the NLSE, for a slightly unstable wave, which is also referred to as the Ginzburg-Landau Equation

$$i\psi_t + \psi_{xx} \pm \left(\beta|\psi|^2 - V\right)\psi = 0 \tag{1.3}$$

Solutions of the LSE in an infinite potential well are found in Quantum Mechanics text books [4]. A nonlinear nonlocal equation describing the evolution of a fluctuating scalar field has been studied [5] and it was found that the structures (and their spectra) observed coincide with the eigenfunctions (and eigenvalues, respectively) of the linear quantum mechanical Schr ö dinger equation. Some work has been done on the NLSE with saddle-like potential the existence of positive, bound states were found. Work on the NLSE in an infinite potential well has not been reported.

The rest of the paper is organized as follows: In section 2, the equations are developed and the methods of solutions are discussed; section 3 deals with the analysis of the results; section 4 discusses the result and section 5 concludes the paper.

2.0 Theoretical Analysis

(a) Numerical Method

If one replaces the potential $V(x)$ in the time dependent one-dimensional LSE by $|\psi|^P$, where ψ is the wave function, one obtains the NLSE

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + |\psi|^P\psi$$

which in units of $\hbar = 1$ gives

$$i\frac{\partial\psi}{\partial t} + \alpha\frac{\partial^2\psi}{\partial x^2} + \beta|\psi|^P\psi = 0; \tag{2.1}$$

where $\alpha = \frac{1}{2m}$ and negative sign is absorbed into β (the nonlinear parameter) which is introduced for generalization. Their effects were also analysed. Give an attractive perturbation $V(x)\psi$ by some external potential equation (2.1) becomes

$$i\frac{\partial\psi}{\partial t} + \alpha\frac{\partial^2\psi}{\partial x^2} + \beta|\psi|^P\psi + V(x)\psi = 0; \tag{2.2}$$

By setting $V(x) = 0$ inside the potential well and assuming a solution of the form [6]

$$\psi = u(x)e^{-i\lambda t} \tag{2.3}$$

in equation (2.2) one gets

$$-\alpha\frac{\partial^2 u}{\partial x^2} + \beta|u|^P u = \lambda u \tag{2.4}$$

Equation (2.4) was solved for the infinite potential well numerically using the shooting method with boundary conditions

$$u(-a) = u(a) = 0 \tag{2.5}$$

This was done by converting the boundary value problem equation (2.5) into an initial value problem (ivp)

$$u(-a) = 0; \quad u'(-a) = 1 \tag{2.6}$$

To obtain an eigenvalue λ equation (2.4) is solved subject to equation (2.6) such that the solution $u(x)$ satisfies $u(a) = 0$. It was found that only certain discrete values of λ satisfy the boundary condition equation (2.5). More than 100 such λ's were obtained but, owing to limited space, only the first 100 are presented in Table 1 for the case in which $\alpha = \beta = a = 1$. The second, third and fourth columns respectively gives the λ's for the NLSE with $p = 2$, the NLSE with $p = 4$ and the LSE. Sketches of the eigenfunctions for the first four λ's are given in Figure1 for the NLSE with $p = 2$. The case $p = 4$ and the LSE are similar. Figure 2 shows the variation of the first eigenvalue λ_1 with power p of the nonlinear term. Figure 3 shows the variation of the fist eigenvalue λ_1 with the nonlinear parameter β. Figure 4 shows the variation of the first eigenvalue λ_1 with the linear parameter α.

(b) **Perturbation method**

According to the numerical result the difference between the eigenvalues of the NLSE and the corresponding eigenvalues of the LSE is small implying that the effect of the nonlinear term, in the NLSE, is small and can be treated as a perturbation to the LSE in a potential well. In this case the Hamiltonian is of the form

$$H = H_0 + H' \tag{2.7}$$

where H_o is the Hamiltonian of the LSE and $H'(\prec\prec H_0)$ is the perturbation which corresponds to the nonlinear term $|\psi|^2$ of the NLSE. The n^{th} eigenvalue E_n of the LSE in an infinite potential well is given by [4]

$$E_n = \frac{\pi^2 \hbar^2 n^2}{8ma^2} \tag{2.8}$$

which in units of $\hbar = 1$ with $a = 1$ and $m = \frac{1}{2}$ (so as to correspond to $\alpha = 1$ in the numerical solution) gives

$$E_n = \frac{\pi^2 n^2}{4} = kn^2 \tag{2.9}$$

where $k = 2.5$. The corresponding eigenfunctions are [7]

$$\psi_n(x) = \sqrt{\frac{1}{a}} \sin\left[n\pi\left(\frac{x}{2a} - \frac{1}{2}\right)\right] \tag{2.10}$$

According to the perturbation method the n^{th} eigenvalue λ_n of the NLSE is given by

$$\lambda_n = E_n + e_n^{(1)} + e_n^{(2)} + \cdots + e_n^{(k)} \tag{2.11}$$

where $e_n^{(k)}$ is the k^{th} order correction of the n^{th} energy level.

$$e_n^{(k)} = \langle \psi | H' | \psi \rangle = \int_{-a}^{a} \psi_n |\psi_n|^2 \psi_n = \frac{1}{a^2} \int_{-a}^{a} \sin^4\left[n\pi\left(\frac{x}{2a} - \frac{1}{2}\right)\right] = \frac{3}{4}$$

for $a = 1$. e_n^2 and higher order correction term vanished. Therefore,

$$\lambda_n = 2 \cdot 5n^2 + 0.75 \tag{2.12}$$

Similarly the corresponding eigenfunctions are given by

$$u_n(x) = \psi_n(x) + v_n^{(1)} + v_n^{(2)} + \cdots + v_n^{(k)} \tag{2.13}$$

where $v_n^{(k)}$ is the k^{th} order correction of the eigenfunction of the n^{th} energy level. However, $v_n^{(k)}$ vanished for all values of k. Hence

$$u_n(x) = \psi_n(x) = \sqrt{\frac{1}{a}} \sin\left[n\pi\left(\frac{x}{2a} - \frac{1}{2}\right)\right].$$

3.0 Analysis of Results

The data of Table 1 was treated in the following was: [8]

1. The graph λ_n versus n is shown in Figure 5. By fitting a curve through the eigenvalues directly i.e. through the graph of Figure 5, one obtained for $p = 2$

$$\lambda_n = 1 - 4\cdot14439\times10^{-2} n + 2\cdot467767n^2 \tag{3.1a}$$

$$\lambda_n = 1 - 0\cdot1787558n + 2\cdot474519n^2 - 7\cdot692831\times10^{-5} n^3 \tag{3.1b}$$

and for $p = 4$

$$\lambda(n) = 1 - 0\cdot03956844n + 2\cdot46773n^2 \tag{3.2a}$$

$$\lambda(n) = 1 - 0\cdot1850615n + 2\cdot474859n^2 - 8\cdot108868\times10^{-5} n^3 \tag{3.2b}$$

2. By finding the first, second and third differences of the λ's one found that the second difference is more or less constant (about 4.9392) and the third difference is almost zero (about 0.0001). This gives a recursive formula for the generation of the λ's as

$$\lambda_{n+2} = 2\lambda_{n+1} - \lambda_n + 4\cdot9392, \text{ for } p = 2 \tag{3.3}$$

$$\lambda_{n+2} = 2\lambda_{n+1} - \lambda_n + 4\cdot9357, \text{ for } p = 4 \tag{3.4}$$

4.0 Discussion of Results

From equations (3.1) and (3.2) it can be seen that the differences between the quadratic and the cubic curves for each of the cases $p = 2$, and $p = 4$ are insignificant, indicating that the λ's are related by a quadratic expression of their energy levels, the n's. The recursive formulae equations (3.3) and (3.4) also justify these relations since by differentiating the quadratic expressions twice with respect to n one gets the constant terms in the recursive formulae.

From Figure 3, it can be seen that the nonlinear term has the effect of increasing the value of the λ's. That is, the higher the nonlinear parameter, β, the higher the value of the λ's. This implies that the NLSE describes self-energising systems such as a laser beam which modifies the dielectric of the medium in which it propagates.

It is observed that as p increases λ_n for the NLSE tend to λ_n for the LSE (see Figure 2 for the case $n = 1$), which means that the effect of the nonlinear term, with fixed β (= 1 in this case) decreases as p increases. This is because the NLSE describes small amplitude waves such that $|u|^p \prec\prec 1$ for $P \succ\succ 1$. The effect of the nonlinear term is also insignificant for large values of λ, in which case the λ's for both the LSE and the NLSE with p = 2, 4, ... coincide; see λ_n for $n \geq 50$ in Table 1. This is because for large λ's the effect of the linear terms in the NLSE dominates that of the nonlinear term such that the equation is essentially linear, with $H' \prec\prec H_0$.

5.0 Conclusion

The following conclusions can be drawn from the analysis:

* The eigenvalues of the NLSE in an infinite potential well are related by a quadratic expression of the energy levels as in the LSE.
* The NLSE describes the evolution of small amplitude waves since as p increases the effect of the nonlinear term, $|u|^p$, decreases.
* The NLSE also describes a self-energising system since the nonlinear term increases the energy eigenvalues.

Table 1: Eigenvalues of the NLSE with p = 2, 4, LSE

n	$p=2$	$p=4$	LSE
1	2.760	2.567	2.460
2	9.940	9.876	9.860
3	22.240	22.208	22.200
4	39.490	39.479	39.470
5	61.690	61.685	61.680
6	88.830	88.827	88.820
7	120.900	120.903	120.900
8	157.910	157.914	157.910
9	199.860	199.859	199.850
10	246.740	246.740	246.740
11	298.550	298.556	298.550
12	355.300	355.306	355.300
13	416.990	416.991	416.990
14	483.610	483.611	483.610
15	555.160	555.165	555.160
16	631.650	631.655	631.650
17	713.080	713.079	713.070
18	799.430	799.438	799.430
19	890.730	890.732	890.730
20	986.960	986.960	986.960
21	1088.120	1088.124	1088.120
22	1194.220	1194.222	1194.220
23	1305.250	1305.255	1305.250
24	1421.220	1421.223	1421.220
25	1542.120	1542.125	1542.120
26	1667.960	1667.963	1667.960
27	1798.730	1798.735	1798.730
28	1934.440	1934.442	1934.440
29	2075.080	2075.084	2075.080
30	2220.660	2220.661	2220.660
31	2371.170	2371.172	2371.170
32	2526.610	2526.619	2526.610
33	2687.000	2687.000	2687.000
34	2852.310	2852.316	2852.310
35	3022.560	3022.566	3022.560
36	3197.750	3197.752	3197.750
37	3377.870	3377.873	3377.870
38	3562.920	3562.928	3562.920
39	3752.910	3752.918	3752.910
40	3947.840	3947.842	3947.840
41	4147.700	4147.702	4147.700
42	4352.490	4352.496	4352.490
43	4562.220	4562.226	4562.220
44	4776.890	4776.890	4776.880
45	4996.480	4996.489	4996.480
46	5221.020	5221.022	5221.020
47	5450.490	5450.491	5450.480
48	5684.890	5684.895	5684.890
49	5924.230	5924.233	5924.220
50	6168.500	6168.506	6168.500
51	6417.710	6417.714	6417.710
52	6671.850	6671.857	6671.850
53	6930.930	6930.935	6930.930
54	7194.940	7194.947	7194.940
55	7463.890	7463.895	7463.880
56	7737.770	7737.777	7737.770
57	8016.590	8016.594	8016.580
58	8300.340	8300.346	8300.330
59	8589.030	8589.033	8589.020
60	8882.650	8882.654	8882.640
61	9181.210	9181.211	9181.190
62	9484.700	9484.703	9484.680
63	9793.120	9793.129	9793.110
64	10106.490	10106.490	10106.470
65	10424.790	10424.790	10424.770
66	10748.020	10748.020	10748.000
67	11076.190	11076.190	11076.160
68	11409.290	11409.290	11409.260
69	11747.320	11747.320	11747.300
70	12090.290	12090.290	12090.260
71	12438.200	12438.200	12438.170
72	12791.040	12791.040	12791.010
73	13148.820	13148.820	13148.780
74	13511.530	13511.530	13511.490
75	13879.170	13879.170	13879.130
76	14251.760	14251.000	14251.710
77	14629.270	14629.270	14629.220
78	15011.720	15011.720	15011.670
79	15399.110	15399.110	15399.050
80	15791.430	15791.430	15791.360
81	16188.690	16188.690	16188.620
82	16590.880	16590.880	16590.800
83	16998.010	16998.010	16997.920
84	17410.070	17410.070	17409.980
85	17827.070	17827.070	17826.970
86	18249.000	18249.760	18248.890
87	18675.860	18675.860	18675.760
88	19107.670	19107.670	19107.550
89	19544.410	19544.410	19544.280
90	19986.080	19986.080	19985.950
91	20432.690	20432.690	20432.550
92	20884.230	20884.230	20884.080
93	21340.710	21340.710	21340.550
94	21802.130	21802.130	21801.950
95	22268.480	22268.480	22268.290
96	22739.760	22739.760	22739.570
97	23215.980	23215.980	23215.770
98	23697.140	23697.140	23696.920
99	24183.230	24183.230	24183.000
100	24674.260	24674.260	24674.010

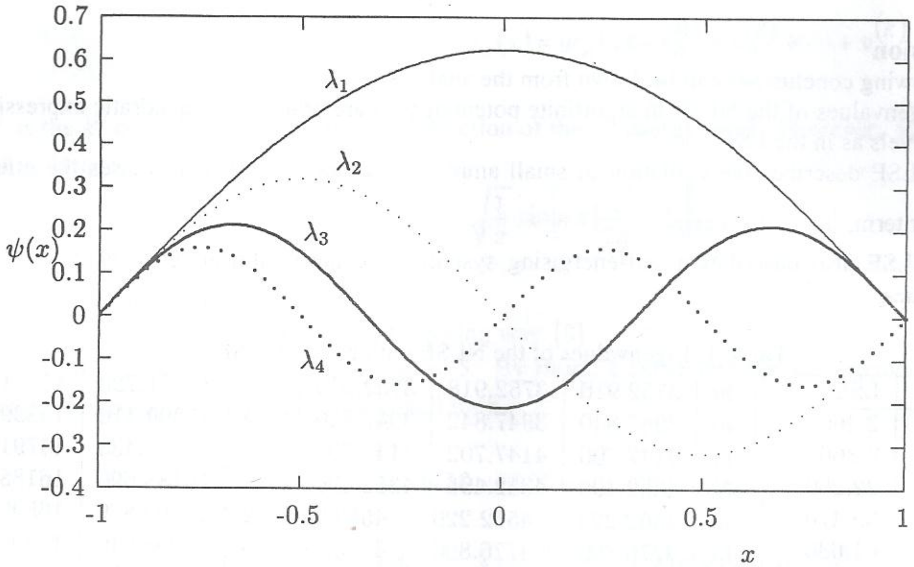

Figure 1: A plot of the eigenfunctions $\psi(x)$ versus x for the first four eigen values: $\lambda_1, \lambda_2, \lambda_3$ and λ_4

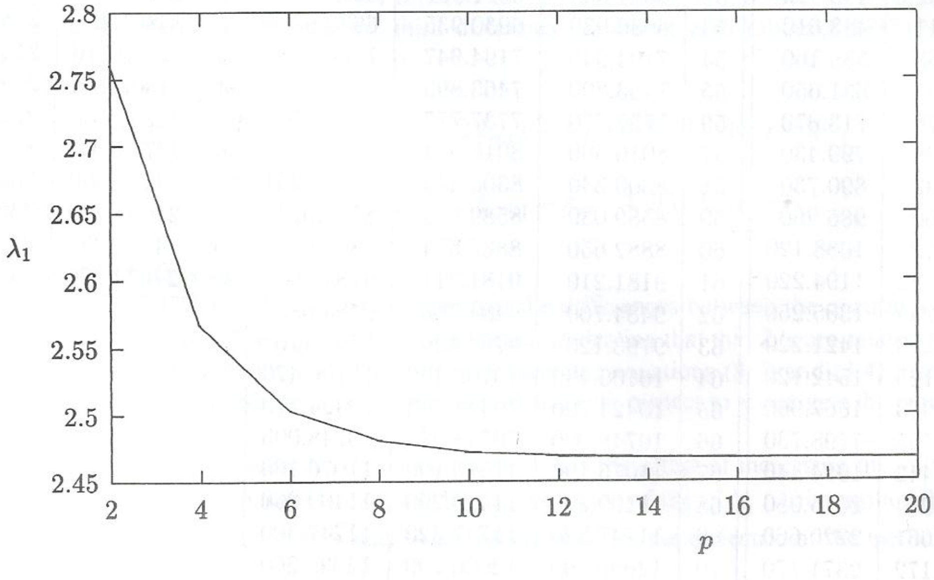

Figure 2: Variation of the first eigenvalue λ_1 with the power p of the nonlinear term

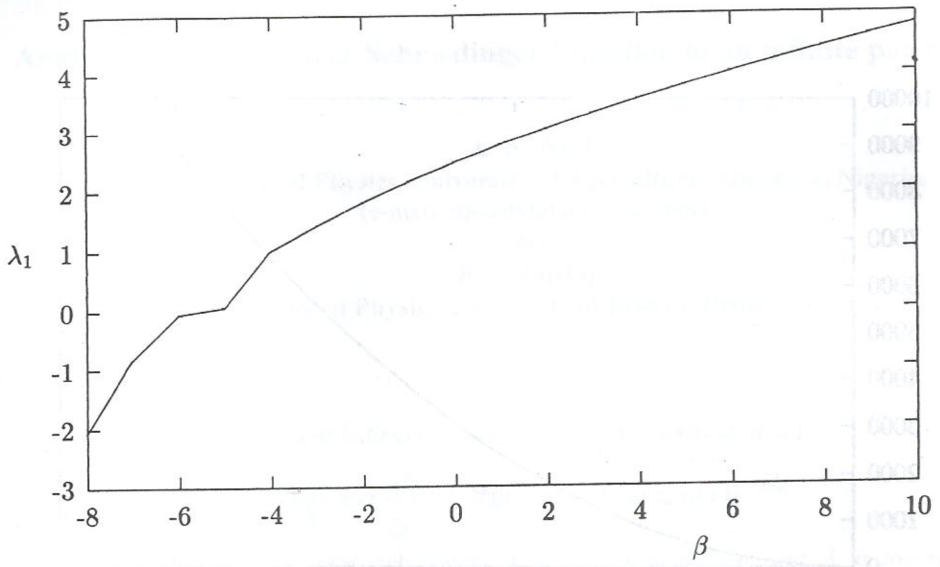

Figure 3: Variation of the first eigenvalue λ_1 with the power *with* the nonlinear parameter β

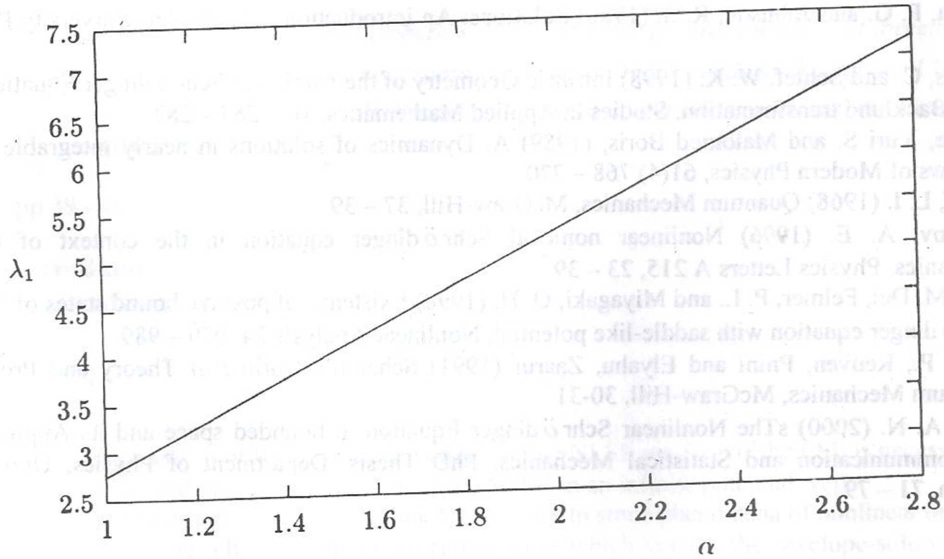

Figure 4: Variation of the first eigenvalue λ_1 with the power *with* the linear parameter α

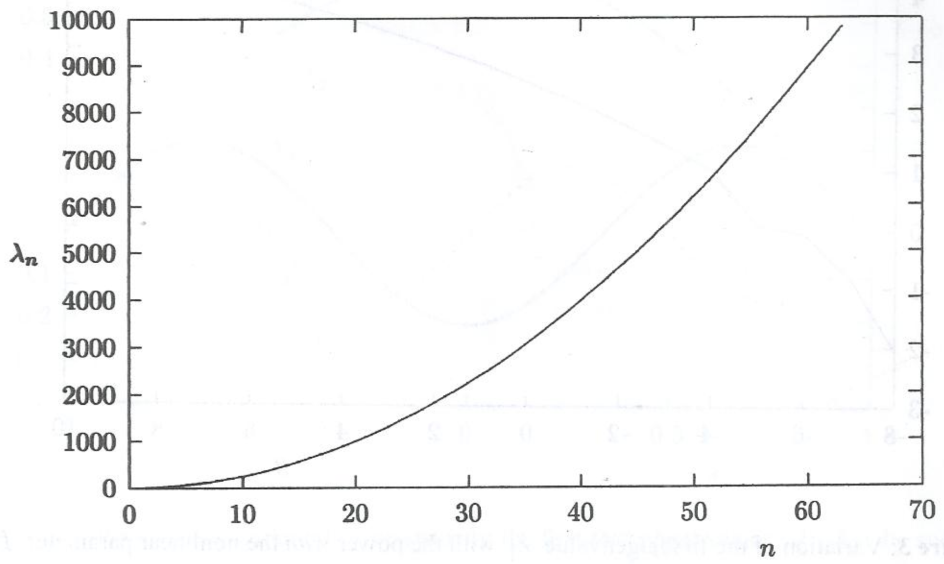

Figure 5: Variation of eigenvalue λ_n's with the energy levels, n's for the NLSE

References

[1] Drazin, P. G. and Johnson, R. S. (1980) Solutions: An introduction. Cambridge University Press, 198 – 200

[2] Rogers, C. and Schief, W. K. (1998) Intrinsic Geometry of the Nonlinear Schr ö dinger Equation and its Auto-Backlund transformation, Studies in Applied Mathematics, 101, 267 – 287

[3] Kivsha, Yuri S. and Malomed Boris, (1989) A. Dynamics of solutions in nearly integrable systems, Reviews of Modern Physics, 61(4) 768 – 770

[4] Schiff, L. I. (1968) Quantum Mechanics, McGraw-Hill, 37 – 39

[5] Filippov, A. E. (1996) Nonlinear nonlocal Schr ö dinger equation in the context of Quantum Mechanics, Physics Letters A 215, 23 – 39

[6] Pino, M. Del, Felmer, P. L. and Miyagaki, O. H. (1998) Existence of positive bound states of Nonlinear Schr ö dinger equation with saddle-like potential, Nonlinear Analysis 34, 979 – 989

[7] Yoav, P., Reuven, Pnini and Elyahu, Zaarur (1991) Schaum's Outline of Theory and Problems of Quantum Mechanics, McGraw-Hill, 30-31

[8] Njah, A. N. (2000) sThe Nonlinear Schr ö dinger Equation in bounded space and its Applications to Telecommunication and Statistical Mechanics, PhD Thesis, Department of Physics, University of Ibadan, 71 – 79