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A Computed Solution to the Schrödinger Equation in the One-Dimensional Non-Relativistic Electron Case Using a Polynomials Expansion Scheme

Ayşe Yumak[1], Karem Boubaker[2, *]

[1]Physics Department, Faculty of Arts and Sciences, Marmara University, Istanbul, Turkey
[2]Unity of Physics of Semi-Conductings Disposals UPDS, Tunis EL MANAR University, Tunisia

Abstract

In this paper, travelling wave solutions to the nonlinearly dispersive Schrödinger equation are computed in the case of one-dimensional non-relativistic electron confined to a cylindrical quantum well. Investigations gave evidence to the possibility of simplified continuous solutions which are in good agreement with the probabilistic interpretation of this equation.

Keywords

Schrödinger Equation, Non-Relativistic Electron, Quantum Well, Boubaker Polynomials Expansion Scheme BPES, Rogue-Langmuir Traveling Wave

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1. Introduction

The well-known nonlinearly dispersive Schrödinger equation [1-8], described as:

$$i\frac{\partial u}{\partial t}+\frac{\partial^2 (u|u|^{n-1})}{\partial x^2}+\mu u|u|^{m-1}=0 \tag{1}$$

where u is the unknown function which determines the probability distribution, μ is a given parameter and m and n are positive integers and denote the intensity of the nonlinear term. This equation arises in a large number of mathematical and engineering problems such fluid mechanics, solid state physics, optic, chemical physics and plasma physics [5-12]. They also successfully represent an important class of nonlinear equations with many applications in updated physical sciences. i. e. for describing pulse propagation with equal mean frequencies in bi-refringent nonlinear fibres.

Exact and analytical solutions for nonlinearly dispersive Schrödinger equation have attracted considerable attention [9-16]. Nevertheless, most of provided standard results of boundary value problems for the nonlinear Schrödinger equation studies were not sufficient to investigate finite geometry configurations since coefficients of the differential equations have been usually chosen such as bounded and measurable functions. Several attempts yielded in this context, families of exact analytical solutions which were obtained using elementary functions [11-14].

In the present work, a polynomial expansion scheme is performed in order to obtain Rogue-Langmuir-type traveling wave solution to Eq. (1). This paper is organized as follows. In Section 2, the resolution protocol is presented along with the studied system patterns.. In Section 3, plots of the are shown ad discussed. Last section is the conclusion.

2. Resolution Protocol

Schrödinger's equation is introduced here in the case of a one-dimensional non-relativistic electron e^- of mass m, moving inside a cylindrical quantum well (C) of radius R (Fig. 1).

* Corresponding author
E-mail address: boubaker_karem@yahoo.com (K. Boubaker)

The potential in the whole space is defined as:

$$\begin{cases} \psi(r)\big|_{r\in[0,R]} = 0; \\ \psi(r) = \infty \quad \text{elsewhere} \end{cases} \tag{2}$$

The situation is such as there is an infinitely high R-radius cylindrical surface at $r = R$ zone .

Schrödinger's equation in cylindrical co-ordinate system for the non-relativistic electron in quantum well is:

$$\frac{\hbar^2}{2m}\frac{\partial^2(u(r,t)|u(r,t)|^{n-1})}{\partial x^2} + i\hbar\frac{\partial u(r,t)}{\partial t} = \frac{u(r,t)}{|u(r,t)|^{1-m}}\psi(r) \tag{3}$$

where $|u|^2$ represents the probability of finding the electron anywhere .

As long as the purpose consists of yielding a Rogue-Langmuir traveling wave solution, an intermediary wave variable θ is introduced so that:

$$x = Et - i\hbar\theta p^{-1} \tag{4}$$

Consequently it comes that:

$$\begin{cases} \frac{\partial}{\partial x}(.) = -\frac{i\hbar}{p}\frac{\partial}{\partial\theta}(.) \\ \frac{\partial^2}{\partial x^2}(.) = -\frac{i\hbar}{p}\frac{\partial^2}{\partial\theta^2}(.) \\ \frac{\partial}{\partial t}(.) = -\frac{i\hbar}{pE}\frac{\partial}{\partial\theta}(.) \end{cases} \tag{5}$$

It comes, for $n = 2$ and $m = 3$, that Eq. (1) alters to:

$$\begin{cases} \left(\frac{p}{\hbar}\right)^2 \frac{d^2 f(\theta)}{d\theta^2} + \left(\frac{E}{\hbar} + \left(\frac{p}{\hbar}\right)^2\right) f(\theta) - \psi(r) f^3(\theta) = 0 \\ f(\theta) = u(x,t)e^{-\frac{i}{\hbar}(px-Et)} = u(x,t)e^{-\theta} \end{cases} \tag{6}$$

According to the problem geometry, we have the trivial condition $|u|_{r>R} = 0$. Consecutively, and starting from the formulation of the Boubaker Polynomials Expansion Scheme BPES [17-33], the expression of the unknown term of the traveling wave solution is proposed as following:

$$f(\theta) = \frac{1}{2N_0}\sum_{k=1}^{N_0} \tilde{\xi}_k \times B_{4k}(\theta\mu_k) \tag{7}$$

where B_{4k} are the 4k-order Boubaker polynomials, μ_k are B_{4k} minimal positive roots [19-36], N_0 is a prefixed integer, and $\tilde{\xi}_k\big|_{k=1..N_0}$ are unknown pondering real coefficients.

According to precedent studies [22-32], Boubaker Polynomials Expansion Scheme BPES protocol ensures validity of spatial boundary conditions prime to the resolution of the main equation.

This particularity of the protocol has been confirmed earlier by Barry *et al.* [30], Agida *et al.* [31], Yildirim *et al.* [32], Kumar [33], Fridjine *et al.* [34] and Benhaliliba *et al.* [35]. In fact these patterns were based on the properties of the Boubaker polynomials [19-33]:

$$\begin{cases} \sum_{q=1}^{N} B_{4q}(x)\Big|_{x=0} = -2N \neq 0; \\ \sum_{q=1}^{N} B_{4q}(x)\Big|_{x=\mu_q} = 0; \end{cases} \tag{8}$$

and:

$$\begin{cases} \sum_{q=1}^{N} \frac{dB_{4q}(x)}{dx}\Big|_{x=0} = 0 \\ \sum_{q=1}^{N} \frac{dB_{4q}(x)}{dx}\Big|_{x=\mu_q} = \sum_{q=1}^{N} H_q \end{cases} \tag{9}$$

$$\text{with:} H_n = B'_{4n}(\mu_n) = \left(\frac{4\mu_n[2-\mu_n^2]\times\sum_{q=1}^{n} B_{4q}^2(\mu_n)}{B_{4(n+1)}(\mu_n)} + 4\mu_n^3\right)$$

By combining the formulation Eq.(6) and that of Eq.(6), we obtain, for the given potential expression $\psi(r)$ in Eq. (2):

$$\left(\frac{p}{\hbar}\right)^2 \sum_{k=1}^{N_0} \xi_k \times \mu_k^2 \frac{d^2 B_{4k}(\theta\mu_k)}{d\theta^2} + \left(\frac{E}{\hbar} + \left(\frac{p}{\hbar}\right)^2\right)\sum_{k=1}^{N_0} \xi_k \times B_{4k}(\theta\mu_k) = 0 \tag{10}$$

The BPES solution is obtained by determining the non-null set of coefficients $\tilde{\xi}_k^{(sol.)}\big|_{k=1..N_0}$ that minimizes the absolute fuctional Λ_{N_0} :

$$\begin{cases} \Lambda_{N_0} = \left|\left(\sum_{k=1}^{N_0} \mu_k^2 \tilde{\xi}_k^{(sol.)} \times \varpi_k\right) + \left(\frac{1}{2N_0}\sum_{k=1}^{N_0} \tilde{\xi}_k^{(sol.)} \times \varpi'_k\right)\right| \\ \text{with:} \end{cases} \tag{11}$$

$$\varpi_k = \frac{p^2}{2\hbar^2 N_0}\oint_{(C)} \left(\frac{d^2 B_{4k}(\theta\mu_k)}{d\theta^2}\right) d\theta$$

and

$$\varpi'_k = \frac{1}{2N_0}\left(\frac{E}{\hbar}+\frac{p^2}{\hbar^2}\right)\oint_{(C)} B_{4k}(\theta\mu_k)\,d\theta$$

Finally the solution of Eq. (3) is:

$$\begin{cases} u^{sol.}(x,t) = \\ \qquad \dfrac{1}{2N_0}\displaystyle\sum_{k=1}^{N_0} \tilde{\xi}_k^{sol.} \times B_{4k}\left(\frac{i}{\hbar}(px-Et)\mu_k\right) e^{-\frac{i}{\hbar}(px-Et)} \\ x\in[0,R], T\in[0,t_m], t_m = 2\pi\hbar/E \end{cases} \quad (12)$$

3. Computed Solution Plots and Patterns

Figure 2 shows plots of the obtained solution, for increasing values of N_0 ($N_0 = 11$, 23 and 43), while Figure 3 corresponds to the convergent solution modulus, obtained for $N_0 > 57$. All the solutions have been represented with $[0,1]$ and $[0,t_m]$ as space and time ranges, respectively.

It may be appropriate to point out that Eq. (3) is derived for short amplitude quasi-stationary slow motion describing the Rogue-Langmuir pondero-motive force. Most of classical solutions, which describe a classical-type particle motion under the action of such forces, consist of linear sums of wave functions corresponding to different energies [39,40] . The present solution accounts for the trapping of such waves in an infinite well, and oppositely to many other results, it concentrates the electron energy into a small region near at the vicinity of the central zone (Fig.4). This paradox can be explained by the nonlinear properties of the medium as well as the abrupt potential discontinuity at the envelop *r*=*R*.

Figure 4 presents the probability distribution within the cylinder (*C*). It monitors a typical single energy wave function having a static probability distribution in good agreement with the results of Banica *et al.* [1], Bégout *et al.* [2], Nadin [4], Gui *et al.* [3], Liu [41], Liang *et al.* [42-43] and Khang *et al.* [41].

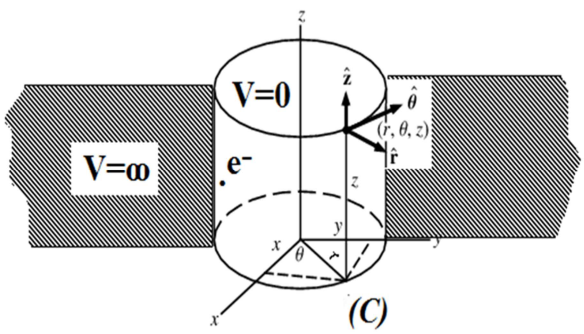

Figure 1. Non-relativistic electron moving inside a cylindrical quantum well

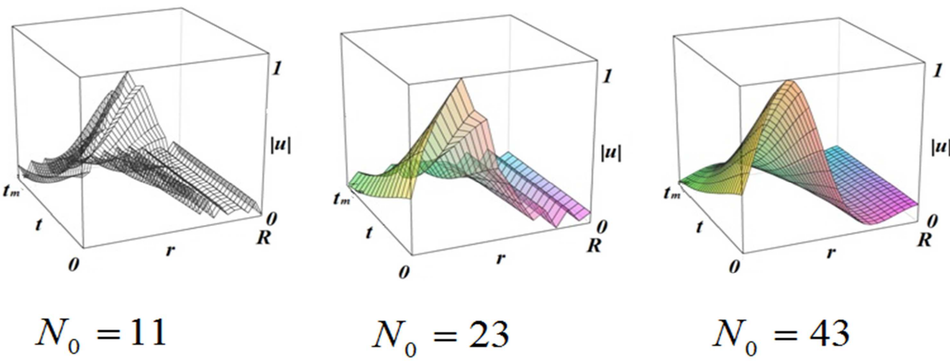

Figure 2. Solution convergence patterns (plots for $N_0 = 11$, 23 and 43)

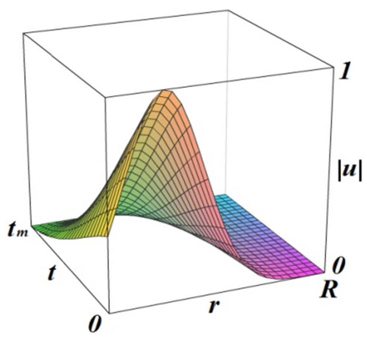

Figure 3. Convergent solution plots for $N_0 > 57$

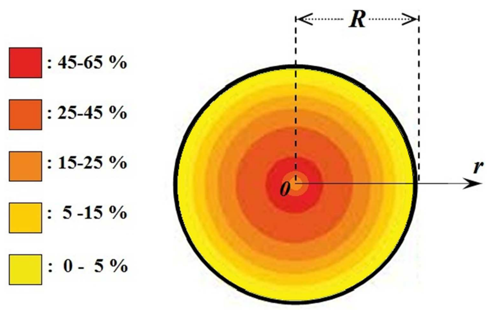

Figure 4. Probability distribution ($|u|^2$)within the cylinder (*C*)

4. Conclusion

In this paper, we have proposed piecewise continuous and uni-modal Rogue-Langmuir-type traveling wave solution to the well known Schrödinger equation. The performed polynomial scheme has ensured the verification of boundary condition in advance to resolution process. The obtained solutions have been expressed in terms of wave function modulus and presented the singular advantage of imposing no quantification for both particle momentum and energy oppositely to most classical solutions. The convergence of the protocol has been discussed and enhanced accordingly.

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