Variational approximations for intersite soliton in a cubic-quintic discrete nonlinear Schrödinger equation

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Abstract. In this paper, the approximation for stationary soliton solution with intersite-typed configuration in the cubic-quintic DNLS equation for anti-continuum limit is determined by a variational approximation (AV) method. The proposed ansatz is of the form an exponential function with three variational parameters. The obtained VA solutions are then examined its validation and compared with the corresponding numerical solutions. The results show that the VA solutions are valid and provide a very good agreement with the numeric.

1. Introduction
One of equations that is often studied in both the theory aspect and in the context of its application is the discrete nonlinear Schrödinger (DNLS) equation. This is because, the equations are modeling many important phenomenal, such as implemented in an experiment as a set of parallel ribs made of a semiconductor material (AlGaAs) [1], a relevant model for a wide range of applications including nonlinear optics (waveguide arrays), matter waves (Bose–Einstein condensates trapped in optical lattices) and molecular biology (modeling the DNA double strand) [2].

The general form of the DNLS equation is given by [2]

\[ i\psi_n = \varepsilon (\psi_{n+1} - 2\psi_n + \psi_{n-1}) + F(\psi_{n+1}, \psi_n, \psi_{n-1}), \]

(1)

where \( \psi_n \equiv \psi_n(t) \in \mathbb{C} \) is a wave function at time \( t \in \mathbb{R}^+ \) and site \( n \in \mathbb{Z} \), \( \psi_n \) represents the derivative of the function \( \psi_n \) with respect to \( t \), \( \varepsilon > 0 \) represents coupling constant and \( F \) form a nonlinear term that has several forms between them:

Cubic

\[ F_{\text{cub}} = |\psi_n|^2 \psi_n. \]

(2)

Quintic

\[ F_{\text{quin}} = |\psi_n|^4 \psi_n. \]

(3)

Ablowitz-Ladik (AL)

\[ F_{\text{AL}} = \frac{1}{2} |\psi_n|^2 (\psi_{n+1} + \psi_{n-1}). \]

(4)

The DNLS equation with nonlinear term cubic (2) and quintic (3) known as non-integrable equation (the solution cannot expression in exact). while 1975-1976, Ablowitz and Ladik [3] showed that the DNLS equation with nonlinear term (4) is integrable. For nonintegrability equations, an analytic approach is needed to approximate the solution. One of the methods which is well known and has been long used to approximate solutions (including the localized states) of a nonlinear evolution equation is
the so-called variational approximation (VA). Formulation of this method is based on theory of Lagrangian and Hamiltonian mechanics (see, e.g., [4]). The success of this method depends heavily on the estimator function (ansatz) used in approaching the desired solution.

VA methods have been used in various equations, including in determining soliton solution in the cubic DNLS equation (3). Aceves et al [5] used the VA method to approximate the onsite soliton solution (which has value maximum on one site). Other than that, VA methods are also applied to approximate an intersite soliton solution (which has value maximum on two site) with a symmetrical configuration by Cuevas et al [6]. Furthermore, Kaup et al [7] developed the VA method formulation to approximate the asymmetric intersite soliton solution. The ansatz function used in [6] and [7] applies for the case $\epsilon \approx 0$ or known as the anti-continuum limit term.

VA results obtained so far have been confirmed for validation through numerical comparisons for certain parameter values. To justify general VA validation, Chong et al. [8] have developed a theorem can be used as a validation of VA results. Chong et al then confirmed that the estimator function for solitons with more parameters many provide a more accurate approximation.

In this paper, the VA method will be applied to determine solution of intersite soliton in the following equation:

$$i\dot{\psi}_n = -C(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - B|\psi_n|^2\psi_n + Q|\psi_n|^4\psi_n, \quad (5)$$

Where $\psi_n(t): \mathbb{R} \rightarrow \mathbb{C}$ and $(C, B, Q)$ are real-valued parameters. Nonlinear Schrödinger lattices have proved to be relevant models in a variety of contexts (see reviews in [8], including the description of optical pulses in one-dimensional waveguide arrays [4]. In this application, the quantity $|\psi_n|^2$ represents the intensity of the electric field of waveguide $n$, $C > 0$ represents coupling strength between adjacent waveguides and $(B, Q)$ measure the nonlinearity strength.

This paper is structured in the following systematics. In Part 2 we discuss the construction of variational approximations. Section 3 discusses the comparison of analytic results with numerical results. Furthermore variational approximation validation is presented in Section 4. Finally, in Section 5 a conclusion is drawn from the results of the study.

2. The Formulation of Variational Approximation

Here are the systematic steps of the VA method [8]:

a) Propose a reasonable trial function (ansatz) which contains a finite number of parameters (called variational parameters).

b) Substitute the proposed ansatz into the Lagrangian and evaluate the resulting sums (for discrete systems) or integrations (for continuous system).

c) Find the critical points of the variational parameters by solving the corresponding Euler-Lagrange equations.

As the first step, the Lagrangian of the system is formulated in advance (5). This is given by the following Lemma.

**Lemma 1.** The lagrangian of equation (5) is given by

$$L = \frac{i}{2} \left( \bar{\psi}_n \psi_n - \psi_n \bar{\psi}_n \right) + C(\bar{\psi}_n \psi_{n+1} + \psi_n \bar{\psi}_{n+1} - 2|\psi_n|^2) + \frac{B}{2} |\psi_n|^4 - \frac{Q}{3} |\psi_n|^6, \quad (6)$$

where $\bar{\psi}_n$ states the conjugate complex of $\psi_n$.

**Proof.** The Euler-Lagrange equation for the system being reviewed is

$$\frac{\partial L}{\partial \psi_n} - \frac{d}{dt} \frac{\partial L}{\partial \psi_n} = 0 \quad (7)$$

The following will show that (5) with Lagrangian (6) will produce equation (5). Note that for an $n = m \in \mathbb{Z}$, equation (6) can be written

$$L = \cdots + \left[ \frac{i}{2} \left( \bar{\psi}_{m-1} \psi_m - \psi_{m-1} \bar{\psi}_m \right) + C(\bar{\psi}_{m-1} \psi_m + \psi_{m-1} \bar{\psi}_m - 2|\psi_{m-1}|^2) + \right. \left. \frac{B}{2} |\psi_{m-1}|^4 - \frac{Q}{3} |\psi_{m-1}|^6 \right] + \left[ \frac{i}{2} \left( \bar{\psi}_m \psi_{m+1} - \psi_m \bar{\psi}_{m+1} \right) + C(\bar{\psi}_m \psi_{m+1} + \psi_m \bar{\psi}_{m+1} - 2|\psi_m|^2) + \right.$$

$$\left. \frac{B}{2} |\psi_m|^4 - \frac{Q}{3} |\psi_m|^6 \right] + \cdots$$
\[ \frac{B}{2} |\psi_m|^4 - \frac{Q}{3} |\psi_m|^6 \] + \ldots

(8)

\[ L \text{ is lowered to } \psi_m \text{ and } L \text{ to } \dot{\psi}_m, \text{ so is obtained} \]
\[ \frac{\partial L}{\partial \psi_m} = C \ddot{\psi}_{m-1} + \frac{i}{2} \ddot{\psi}_m + C \ddot{\psi}_{m+1} - 2C \ddot{\psi}_m + B \ddot{\psi}_m^2 - Q(\psi_m \ddot{\psi}_m)^2 \ddot{\psi}_m. \]

(9)

\[ \frac{\partial L}{\partial \ddot{\psi}_m} = \frac{i}{2} \ddot{\psi}_m \Rightarrow \frac{d}{dt} \frac{\partial L}{\partial \psi_m} = \frac{i}{2} \ddot{\psi}_m. \]

(10)

Cause \[ \ddot{\psi}_m \psi_m = |\psi_m|^2 \] so equation (7) become
\[ -i \ddot{\psi}_m = -C (\ddot{\psi}_{m-1} - \ddot{\psi}_m - \ddot{\psi}_{m+1}) - B |\psi_m|^2 \ddot{\psi}_m + Q |\psi_m|^4 \ddot{\psi}_m. \]

(11)

The conjugate is applied on both sides of equation (11), then multiplied by -1 and replaced by \( m = n \), then it is obtained
\[ i \ddot{\psi}_n = -C (\ddot{\psi}_{n+1} - 2 \ddot{\psi}_n - \ddot{\psi}_{n-1}) - B |\psi_n|^2 \ddot{\psi}_n + Q |\psi_n|^4 \psi_n. \]

(12)

Which is equation (5).

Stationary discrete soliton solutions can be obtained by substituting \( \psi_n(t) = u_n e^{-i \mu t} \), where \( \mu \) represents the oscillation frequency, to DNLS (5) so it is obtained
\[ -C (u_{n+1} - 2 u_n + u_{n-1}) - B |u_n|^2 u_n + Q |u_n|^4 u_n - \mu u_n = 0. \]

(13)

In general the solution \( u_n \) is complex, but analysis of equation (13) for discrete soliton, which fulfills \( u_n \to 0 \) when \( n \to \pm \infty \), can be simplified without reducing the generality by reviewing only real value solutions [9]. Thus equation (11) becomes
\[ -C (u_{n+1} - 2 u_n + u_{n-1}) - B u_n^3 + Q u_n^5 - \mu u_n = 0. \]

(14)

In this case, there are infinite number of configurations for discrete solitons, but in this paper only intersite soliton solutions are reviewed, which are centered on two sites.

In the second step, choose the appropriate ansatz function, which contains a number of parameters. In estimating a stationary intersite soliton in the cubic-quintic DNLS equation (13), Chong et al. [8] proposed the following anzatz function:
\[ u_n = A e^{-\eta (n-\frac{1}{2})}, \]

(15)

where \( A \) and \( \eta \) are the variational parameters which respectively state the amplitude and width of the soliton.

In this paper the following ansatz function is selected:
\[ u_n = \begin{cases} A e^{-\eta (n+1)}, & n \leq -1, \\ A e^{-\eta (n+1)}, & n \geq 2, \\ E, & n = 0. \end{cases} \]

(16)

where parameters \( A \) and \( E \) represent the soliton amplitude on site \( n \neq 0 \) and \( n = 0 \) is expected to accommodate the soliton profile which narrows to site \( n = 0 \) and \( n = 1 \) when \( C \to 0 \). Compared to the proposed ansatz Chong (15), ansatz (16), it is expected to improve the accuracy of the variational approximation in the case of the anti-continuum limit.
The third step is to substitute ansatz (16) into the Lagrangian stationary section (6), then complete the sum. This sum is called effective Lagrangian. Using Maple’s help, effective Lagrangian was obtained

\[ L_{\text{eff}} = -\frac{1}{\beta(\epsilon^{\eta} - 1)(\epsilon^{\eta} + 1)} \left( 12CAE - 2e^{2\eta}E^6Q + 2A^6Qe^{6\eta} + 2A^6Qe^{8\eta} - A^2\mu e^{6\eta} + 2Qe^6e^{6\eta} - 24A^2Ce^8\eta + 12CAE^6\eta + 2Qe^6e^{8\eta} + 2Qe^6e^{8\eta} - 3BE^4e^{6\eta} - 3BE^4e^{8\eta} - 12A^2C e^{8\eta} - 3BE^4e^{8\eta} + 12A^2C e^{8\eta} + 6A^2e^{2\eta} \mu + 3BE^4 - 3A^4Be^{8\eta} - 3BA^4e^{4\eta} + 6e^2\mu e^{8\eta} + 6CE^2e^6\eta - 24A^2Ce^{8\eta} - 6E^2e^{8\eta} \mu - 4CAE + 2e^2\mu e^{8\eta} - \frac{2}{3}e^{6\eta}A^6Q + 8e^{8\eta}A^2C + 4e^{6\eta}AE - 4CAe^{8\eta} + 4ACe^8\eta + 2A^2\mu e^{8\eta} + \frac{2}{3}e^{8\eta}A^6Q + e^{6\eta}A^4B - BE^4 e^{2\eta} - \frac{2}{3}Qe^6e^{8\eta} - 8CA^2e^{6\eta} + 4A^2\mu e^{8\eta} - 8A^2Ce^{4\eta} + \frac{2}{3}e^{8\eta}Qe^{2\eta} \right). \]

(17)

Based on the variational principle, the Lagrangian effectively reaches the critical value in the Euler-Lagrange equation. For stationary cases, this yields

\[ \frac{\partial L_{\text{eff}}}{\partial A} = \frac{\partial L_{\text{eff}}}{\partial E} = \frac{\partial L_{\text{eff}}}{\partial \eta} = 0. \]

(18)

By substituting effective Lagrangian (17) to equation (18), the following variational equation system is obtained:

\[ A_1 + A_2 + A_3 = 0, \]

(19)

\[ B_1 + B_2 + B_3 + B_4 = 0, \]

(20)

\[ C_1 = 0, \]

(21)

where

\[ A_1 = 4Ae^{2\eta} \mu + 8AC e^{\eta} - 4CE e^{2\eta} + 16AC e^{5\eta} + 4e^{8\eta}A^2B + 8A\mu e^{4\eta} - 16AC e^{4\eta}, \]

\[ A_2 = -4e^{6\eta}A^2Q - 8AC e^{2\eta} + 8e^{8\eta}A\mu + e^{6\eta}A^3B - 4e^{8\eta}A^5Q + 8A\mu e^{4\eta} + 4CE e^{8\eta}, \]

\[ A_3 = -8e^{8\eta}AG + 4A^3 e^{6\eta}B - 16ACe^{6\eta} + 8A^3e^{7\eta} - 4CE + 16Ae^{3\eta}C + 4CAe^{6\eta}, \]

\[ B_1 = 4e^{\eta}A^2(-A^2e^{3\eta})B - C + 16Ce^{5\eta} - 12Ce^{4\eta} - 18e^{8\eta}C - 18Ce^{6\eta} - 12Ce^{10\eta}, \]

\[ B_2 = 4e^{\eta}A^2(-2A^2e^{2\eta}B - e^9\mu) - e^{13\eta} - 3e^{7\eta}A^2B - e^{11\eta}A^2B - 5C e^{2\eta} - 8\mu e^{9\eta}, \]

\[ B_3 = 4e^{\eta}A^2(3e^{3\eta}C + e^{5\eta}Q^4Q - 4\mu e^{11\eta} - C e^{14\eta} + 16Ce^{9\eta} + 8Ce^{11\eta} - 2Ce^{7\eta} + 2e^{5\eta}A^2B, \]

\[ B_4 = 20Ce^{7\eta} - 5Ce^{12\eta} - 4\mu e^{3\eta} + 2Ce^{13\eta} - 8\mu e^{5\eta} - 10e^{7\eta}\mu + 2e^{7\eta}A^2Q + QA^4 e^{9\eta}, \]

\[ C_1 = -4CE + 4BE^3 + 4E\mu - 4Qe^5 + 4CA. \]

The final step is to determine the critical points for variational parameters. Because of the complexity of the calculation, the variational parameter values A, E, \eta are obtained as a solution of the systems equation (19) - (21) for the values C, B, Q, \mu given can be calculated numerically using the Newton-Raphson method.

3. The VA Result and Comparisons with Numerics

In this section the results obtained using the AV method will be compared with numerical results. Because of the stationary case, the numerical solution for intersite soliton is obtained from equation (13). Here a numerical solution is determined using the Newton-Raphson method which is calculated on the domains n \in [-N, N], with a large N \in Z. Because solitons have asymptotic tails to zero and one, in the numerical scheme \( u_{\pm(N+1)} = u_{\pm(N)} \) boundary conditions are used.
Figure 1. Comparison of intersite soliton solutions obtained numerically (round-line) and variational approximations (cross-lines) for some values of C, B, Q, and $\mu$. 
In Figure 1 we can observe that the intersite soliton for increasing C value causes the amplitude of the solitons to increase. Likewise, when the Q value increases, the soliton amplitude increases as well. Besides that, it can also be observed that the solution of the variable approximation is more accurate for C and Q which are getting smaller.

4. Validation of VA

Validation of the approximation results for discrete solitons in the DNLS equation (16) is based on Lemma 1 on Chong et al. [8]. To measure the accuracy of the variational solution of the DNLS equation (13), define it

\[ R_n(u) = -C(u_{n+1} - 2u_n + u_{n-1}) - Bu_n^3 + Qu_n^5 - \mu u_n. \] \hspace{1cm} (22)

Note that if \( Q \) are exact solution, then \( R_n(u) \) will be zero for every \( n \). Thus a variational solution will approach an exact solution if \( R_n(u) \to 0 \) for every \( n \).

Validation of the variational approximation to the intersite soliton in the stationary –quintic cubic DNLS equation (13) is given in the following propositions.

**Proposition 1.** Suppose \( u_n \) is the soliton onsite variational solution of the stationary cubic-quintic SNLD equation (13) expressed by ansatz (16) where the variational parameters \( \eta, A, E \) satisfy the equation (19), (20), (21). Then there is \( C_0, K > 0 \) such that for each \( C \in (0, C_0) \), the stationary cubic-quintic SNLD equation (13) has a solution that satisfies

\[ \|u - u_n\| \leq KC^4. \] \hspace{1cm} (23)

**Proof.** Note that the rate of exponential discrete decrease in soliton meets linear theory of different equations, so the solution for the \( \eta \) parameter can be obtained by substituting \( u_n = pe^{-\eta n} \), where \( p \) is a non-zero constant, to the linear part of equation (22), that is

\[ -C(\psi_{n+1} - 2\psi_n + \psi_{n-1}) - \mu u_n = 0 \] \hspace{1cm} (24)

So it is obtained

\[ -C(e^{-\eta} + e^{\eta}) = 2C - \mu \Rightarrow \eta = \text{arccosh} \left(\frac{2C - \mu}{2C}\right). \] \hspace{1cm} (25)

Taylor expansion from \( e^\eta \) at \( \varepsilon \approx 0 \) given by

\[ e^\eta = \frac{C}{\mu} - 2 \frac{C^2}{\mu^2} + 5 \frac{C^3}{\mu^3} - 14 \frac{C^4}{\mu^4} + 42 \frac{C^5}{4} + O(C^6). \] \hspace{1cm} (26)

Then suppose that parameters \( A \) and \( E \) can be written in the form of expansion

\[ A = a_0 + a_1 C + a_2 C^2 + a_3 C^3 + O(C^4), \] \hspace{1cm} (27)

\[ E = b_0 + b_1 C + b_2 C^2 + b_3 C^3 + O(C^4), \] \hspace{1cm} (28)

where \( a_i \) dan \( b_i \) are coefficients that can be found in value by substituting equations (26), (27) and (28) into equations (19) and (20), then collect the terms according to rank \( C \).

Furthermore, substitution of ansatz (16) into equation (22), is obtained

\[ R_n(u) = \begin{cases} \[A(-Ce^{-\eta(n+2)} + 2Ce^{-\eta(n+1)} - Ce^{\eta(n)} - BA^2 e^{3\eta(n+1)} + \frac{QA^4 e^{5\eta(n+1)} - \mu e^{\eta(n+1)}}{n \leq -2} + \frac{-Ce + 2CA - CAe^{-\eta} - BA^3 + QA^5 - \mu A}{n = -1} + \frac{CE - CA - BE^3 + QE^5 - \mu E}{n = 0} + \frac{-CE + 2CA - CAe^{-\eta} - BA^3 - QA^5 - \mu A}{n = 1} + \frac{A(-Ce^{-\eta(n-1)} + 2Ce^{-\eta(n-2)} - Ce^{\eta(n-3)} - BA^2 e^{-3\eta(n-1)} + \frac{QA^4 e^{-\eta(n-1)} - \mu e^{-\eta(n-1)}}{n \geq 2} + \frac{-CE + 2CA - CAe^{-\eta} - BA^3 - QA^5 - \mu A}{n = 1})}{n = 0} + \frac{A(-Ce^{-\eta(n-1)} + 2Ce^{-\eta(n-2)} - Ce^{\eta(n-3)} - BA^2 e^{-3\eta(n-1)} + \frac{QA^4 e^{-\eta(n-1)} - \mu e^{-\eta(n-1)}}{n \geq 2}}\end{cases} + \frac{-CE + 2CA - CAe^{-\eta} - BA^3 - QA^5 - \mu A}{n = 1})\end{cases}\] \hspace{1cm} (29)

Substitution ekspansi (26), (27), (28) to equation (29), so it is obtained

\[ R_{|n|\leq-2}(u) = O(C^3|n|), \]
\[
R_{|n|=1}(u) = O(C^4), \\
R_{n=0,1}(u) = 0, \\
R_{|n|\geq 2}(u) = O(C^{3|n|}).
\]

Notice that sequence \( \{R_i(u)\}_{i=1}^{\infty} \) convergent to 0. So that \(|R_1|^2 + |R_2|^2 + \cdots \) convergent or \( \sum_{i=1}^{\infty} |x_i|^2 < \infty \). This explain that \( R_i(u) \) is in space \( l_2 \) with norm \( \|R(u)\|_{l_2} = \sqrt{|R_1|^2 + |R_2|^2 + \cdots} \), so that (30) is obtained

\[
\|R(u)\|_{l_2} = O(C^4) \text{ when } C \to 0.
\]

Then suppose \( S = \{0\}, e_0 = (\ldots, 0, 0, 0, 1, 0, 0, 0, \ldots) \), and \( e_1 = (\ldots, 0, 0, 0, 1, 0, 0, 0, \ldots) \), for \( c > 0 \). For the intersite discrete solution case, solution \( u \), state by ansatz (16) can be shown to satisfy the relation

\[
\lim_{C \to 0} \|u - u_* - \sigma_0 e_0 + \sigma_1 e_1\|_{l_2} = 0.
\]

Based of Lemma 1 on Chong et al [8], there is \( C_0, K > 0 \) and the single solution \( u \) of the stationary cubic-quintic SNLD equation (13) with \( C \in (0, C_0) \) so that

\[
\|u - u_*\|_{l_2} \leq KC^4.
\]

Because the exact solution is unknown, in practice the quantity of \( \|u - u_*\|_{l_2} \) can be approached by

\[
\text{error} = \|u_{\text{num}} - u_*\|,
\]

where \( u_{\text{num}} \) is numeric solution and \( u_* \) is variational solution.

As an illustration, suppose that the variational solution validation will be checked for the parameter value \( B = 2, \mu = -2 \) with \( Q = 0.2 \) and \( Q = 0.4 \). The error plot (34) of \( C \) for the is given in Figure 2.

Figure 2. Error value between variational and numerical solutions for \( C \) for \( \mu = 0.5, B = 2 \) and \( Q = 0.1 \) (left) dan \( Q = 0.8 \) (right).

From the picture it can be seen that the error value gets bigger when \( C \) enlarges. To find out the function of the error curve, best power fit is performed, which gives the results \( f(C) = 0.00041938C^{5.6286} \) (for \( Q = 0.2 \)) and \( f(C) = 0.00081371C^{5.7913} \) (for \( Q = 0.4 \)). Note that these results satisfy equation (33) in Proposition 1. This confirms that the AV solution for intersite soliton using ansatz (14) is valid.

To compare these results with AV results obtained from ansatz Chong (15), by doing the same calculation as before, look for \( \|R_n(u)\|_{l_2} \) with \( u \) is ansatz (16), then plot the error between numerical and variational solutions as defined in equation (34). Variational calculation results provide

\[
\|R_n u\|_{l_2} = O(C^2)
\]

and the error plot is given in Figure 3 for \( \mu = -0.5, B = 2 \) and \( Q = 0.1 \). From equation (35) and Figure 3 it can be concluded that variational solutions obtained from ansatz (16) are more accurate than ansatz Chong (15). By using the best power fit for the error curve in Figure 3, it is obtained \( f(C) = 0.011872C^{3.097} \).
Figure 3. Error value between variational solutions and numerical solutions to $C$ for $\mu = -0.5$, $B = 2Q$ value, which is $Q = 0.1$.

5. Conclusion
In this paper, we have developed a variational formulation for approximation of the stationary intersite soliton governed by the parametrically cubic quintic discrete nonlinear Schrödinger equation. An ansatz that can deal with anticontinuum limit case has been proposed. The comparison between the analytical result and the corresponding numerical findings showed that our theoretical predictions are very good for small coupling constant $C$ where the accuracy is getting better for larger parametric cubic quintic $B$. However, one should notice that the proposed ansatz (16) cannot capture the smooth growth of the onsite solitons as $C$ increases. Therefore, the better ansatz for this case should be developed and the heuristic validity must be performed rigorously. These interesting problems can be proposed as future study.

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