An efficient determination of critical parameters of nonlinear Schrödinger equation with a point-like potential using generalized polynomial chaos methods

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We consider the nonlinear Schrödinger equation with a point-like source term. The soliton interaction with such a singular potential yields a critical solution behavior. That is, for the given value of the potential strength and the soliton amplitude, there exists a critical velocity of the initial soliton solution, around which the solution is either trapped by or transmitted through the potential. In this paper, we propose an efficient method for finding such a critical velocity by using the generalized polynomial chaos (gPC) method. For the proposed method, we assume that the soliton velocity is a random variable and expand the solution in the random space using orthogonal polynomials. Then the gPC method is used with spectral convergence. The proposed method is expected to find the critical velocity accurately with spectral convergence. Thus the computational complexity is much reduced. Numerical results for the smaller and higher values of the potential strength confirm the spectral convergence of the proposed method.

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1. Introduction

The Nonlinear Schrödinger equation (NLSE) describes a broad range of physical phenomena, e.g. nonlinear modulation of collisionless plasma waves [1], self trapping of a light beam in a color dispersive system [3], helical motion in a very thin vortex filament [13], propagation of heat pulses in an-harmonic crystals [8], modulation instability in water waves [13], etc. In optical fibers, the soliton solutions of the NLSE provide a secure means to carry bits of information over many thousands of miles [3]. Term as the Gross–Pitaevskii equation, the NLSE with an appropriate potential can be utilized to describe the dynamics of the Bose–Einstein condensate, both with the attractive and repulsive nonlinearities [13,21]. Malomed and others studied the dynamics of a $\Phi^4$ kink with additional terms by perturbation theory [22]. An important class of models is formulated in terms of the couple-mode equation for Bragg gratings, with delta-functional defects [20]. An extension of this type of the models leads to complex Ginzburg–Landau equations with the localized gain and nonlocality [25]. Also the scattering of a quantum particle by a potential which includes a delta-function and whose amplitude is nonlinear in the wave function was studied in [23].

Our objective in this paper is to solve the Gross–Pitaevskii equation equipped with a point-like potential to find the critical values of the soliton velocities when the amplitude of the point-like potential is either very small ($\sim 10^{-1}$–$10^{-2}$) or large ($\sim 2.5$–$4.5$) compared with the soliton amplitude which is the unity in our paper.

We know that the soliton solution of the homogeneous NLSE...
\[ i \partial_t u + \frac{1}{2} \partial_x^2 u + u |u|^2 = 0, \quad -\infty < x < \infty, \quad t > 0, \]

with the initial condition \( u_0 \) given by

\[ u_0(x) = A \text{sech}(A(x)) e^{i(x+Vx)} \]

is given by

\[ u(x, t) = A \text{sech}(A(x - Vt)) \exp \left( i \phi + iVx + \frac{i}{2} (A^2 - V^2)t \right), \quad A > 0, \quad V \in \mathbb{R}, \]

where \( A \) is the soliton amplitude, \( V \) is the soliton velocity, and \( \phi \) is the phase lag. Consider a perturbed NLSE, that is, the Gross–Pitaevskii equation by adding an external potential, \(-\epsilon \delta(x)u\),

\[ \begin{cases} i \partial_t u + \frac{1}{2} \partial_x^2 u + u |u|^2 = -\epsilon \delta(x)u, \\ u(x, 0) = u_0(x), \end{cases} \]

where \( \delta(x) \) is the Dirac \( \delta \)-function with a constant \( \epsilon \in \mathbb{R} \). Such an external potential represents the impurity or defect in the optical fiber. The well-posedness of the equation

\[ \begin{cases} i \partial_t u + \frac{1}{2} \partial_x^2 u + u |u|^{p-1} = -\epsilon \delta(x)u, \\ u(x, 0) = u_0(x), \end{cases} \]

with \( p \geq 1 \) and the initial data \( u_0 \) in \( H^1(\mathbb{R}) \), has been extensively studied and is based on the knowledge of the self-adjoint (in \( L^2 \)) operator \(-\partial_{xx} + \epsilon \delta\). Using [5], Le Coz et al. proved the existence of a time \( T > 0 \) and of a unique solution to Eq. (4) (where \( p = 3 \) in \( C([0, T], H^1(\mathbb{R})) \cap C^1([0, T], H^{-1}(\mathbb{R})) \)) satisfying \( \lim_{t \to T} \| \partial_t u \|_2 = \infty \). Moreover, the energy is conserved in time. This result was extended to \( p \geq 1 \) by Fukuizumi et al. in [11]. For \( p = 3 \) (more generally \( p \in (1, 5) \)), global existence in \( H^1 \) also holds by Gagliardo–Nirenberg’s inequality and energy conservation. Global existence in \( H^1 \) is also discussed by Goodman et al. [12] using a fixed-point argument and time-invariance of the \( L^2 \)-norm and of the Hamiltonian derived from the NLSE. Notice that the study of stability of nonlinear bound states which are solutions of the form \( \exp(-i\lambda t)\phi_\omega(x) \) with \( \omega > 0 \), and for which:

\[ -\frac{1}{2} \partial_{xx} \phi_\omega - \epsilon \phi_\omega - |\phi_\omega|^2 \phi_\omega = \omega \phi_\omega \]

plays an important role in the theory of NLSE with defect and could possibly be useful numerically. Explicit formulas and stability analysis for \( \phi_\omega \) can be found in [11,19].

If we now take a soliton approaching the impurity from the left as an initial condition \( u_0 \):

\[ u_0(x) = A \text{sech}(A(x - x_0)) e^{i(x+Vx)}, \quad x_0 \ll 0, \]

then until the time \( t_0 = \frac{x_0}{V} \), the solution will still be given by Eq. (3). In this paper we consider \( A = 1 \) and \( \phi = 0 \). Thus the soliton velocity \( V \) and the strength of the impurity \( \epsilon \) are the only parameters of the problem.

For \( t_0 > \frac{x_0}{V} \), the effects of the potential are highly visible and a lot of research has been done on the transmission and reflection coefficients of the \( \delta \)-potential by the standard scattering theory [15]. Malomed and his co-workers [4,21] showed mainly numerically, that for any given velocity \( V (> 0) \), there exists a threshold value \( \epsilon_{thr} (> 0) \) of \( \epsilon \), for which the soliton can marginally pass through the defect. So for the given velocity \( V \), if \( \epsilon < \epsilon_{thr} \), the soliton can pass through the defect and the soliton gets trapped otherwise. They considered the soliton–soliton collisions within the coupled NLSE. For PDEs from nonlinear optics, a similar phenomenon has been found and studied, e.g. the sine-Gordon equation or nonlinear Schrödinger condensates loaded into optical lattice [9]. In the limiting condition one soliton has very large amplitude and is very narrow accordingly, while the order soliton has finite amplitude and broader width. In this limiting condition the two coupled NLSE are reduced to a single equation, in which the narrow soliton will be represented by the \( \delta \)-function:

\[ i \partial_t u + \frac{1}{2} \partial_x^2 u + u |u|^2 = -\epsilon \delta(x)u. \]

Holmer and his co-workers studied the NLSE with \( V \gg 1 [16] \) and \( V \ll 1, \epsilon \ll 1 [17] \). They showed that for high \( V \), there exits the bound state which is given by

\[ u(x, t) = e^{i\lambda^2/4} \lambda \text{sech}(\lambda |x| + \tanh^{-1}(\epsilon/\lambda)), \quad 0 < \lambda < \epsilon, \]

and this bound state is “left behind” after the interaction (see the bottom right figure of Fig. 4). Also they proved in [17] that for \( V \ll 1 \) and \( \epsilon \ll 1 \), the solution can be approximated by the soliton solution of the homogeneous NLSE (\( \epsilon = 0 \)). To solve Eq. (4) for any given \( \epsilon (> 0) \) and \( V (> 0) \), we consider three cases: (a) small value of \( \epsilon \), where \( \epsilon \leq 0.3 \), (b) moderate
value of $\epsilon$, where $0.3 < \epsilon < 3.5$ [4] and (c) large value of $\epsilon$, where $\epsilon > 3.5$. For solving Eq. (4), one can use the Split Step Fourier Method (SSFM) to reduce the computational time. To get $\epsilon_{th}$ for any given $V$ with certain accuracy one must conduct a series of simulations. The number of simulations increases with the increase of the level of accuracy. In addition to conduct a series of simulations with small time steps, one needs a large amount of the computational time. This is our main motivation to propose a suitable method to overcome such a high computational complexity by using the generalized polynomial chaos (gPC) methods [26].

The gPC method belongs to the class of non-sampling methods [27,28,30]. In this method the stochastic quantities are expanded by orthogonal polynomials. Different types of orthogonal polynomials can be chosen for better convergence. The gPC expansion is a spectral representation in random space and exhibits fast convergence when the expanded function depends smoothly on the random parameters [14,26]. When the gPC method is applied to solve a differential equation, the main computational work is needed to solve the expansion coefficients of the gPC expansion. A common approach is the Galerkin method that minimizes the residue in the polynomial space [26,31]. The stochastic Galerkin (SG) approach, however, would be extremely difficult to use when the governing stochastic equations take complicated forms. In our case, the NLSE contains the nonlinear term $|u|^2 u$. For the SG method, it is very hard to get the corresponding explicit deterministic equations after expanding the nonlinear terms. Thus in this work we use the high-order stochastic collocation (SC) approach [27,29] that combines the advantages of both the Monte Carlo and the gPC-Galerkin methods. The gPC method reduces the number of simulations for finding the critical velocity, $V_c$, for any given value of $\epsilon$ thanks to the high-order convergence of the method. Since the equation has only two parameters, i.e. $\epsilon$ and $V$, we treat at least one of them as a stochastic variable in the gPC framework. In the present work we consider $V$ as the stochastic variable and let $\epsilon$ be fixed. We note that the reduced problem is deterministic and the gPC method, in this work, is used to solve efficiently the deterministic problem. For any given $\epsilon$, we find $V_c$, the critical value of $V$ around which the soliton is either transmitted or trapped. Thus it is obvious that for $V > V_c$, the soliton passes through the defect. By adopting this idea we develop a step-by-step gPC collocation method to find the critical velocity of the soliton.

In [4] the relation between $\epsilon_{th}$ and $V$ was obtained only for the moderate values of $\epsilon$, i.e. for those comparable to the soliton amplitude $A = 1$. But the results of the numerical simulations for very small or large values of $V$ were not obtained, perhaps due to the huge computational burden. By the gPC method, we were able to reduce the overhead computational time of having detailed simulations performed for large and small values of $\epsilon$ to find the corresponding critical velocity $V_c$.

Since the analysis for the moderate values of $\epsilon$ is already done [4], we do not intended to repeat the analysis for those values of $\epsilon$ in this paper. Here we mainly focus on the small and high values of $\epsilon$. For the small values of $\epsilon$, the gPC takes much longer time than the gPC method for the large values of $\epsilon$ due to the extremely small critical velocities.

This paper is organized as follows. In Section 2, we discuss the SSFM. Section 3 describes the gPC collocation method. Section 4 contains the gPC collocation algorithm for the NLSE with the singular potential term to detect the critical velocity $V_c$. Section 5 presents the numerical results. Concluding remarks and future works are presented in Section 6.

2. Split step Fourier method

The SSFM is a pseudo-spectral numerical method used to solve the nonlinear PDEs such as the NLSE. Eq. (1) can be rewritten as

$$\frac{\partial u}{\partial t} = i(N + D)u,$$

where $D = \frac{1}{2} \frac{\partial^2}{\partial x^2}$ and $N = |u|^2$. The solution of Eq. (8) can be formally written as

$$u(x, t) = e^{it(N + D)}u(x, 0),$$

where $u(x, 0)$ is the initial condition. Operators $D$ and $N$ do not necessarily commute. However the Baker–Hausdorff formula can be applied to show that the error will be of order $dt^2$ if we take a small but finite time step $dt$ [24]. We therefore can write

$$u(x, t + dt) \approx e^{iN dt} e^{iD dt} u(x, t).$$

The part of this equation involving $N$ can be computed directly using the wave function $u(x, t)$ at time $t$. To compute the exponential involving $D$ we use the fact that in the frequency domain, the partial derivative operator $\frac{\partial}{\partial x}$ is converted into $ik$, where $k$ is the frequency associated with the Fourier transform. Then we take the Fourier transform of $u(x, t)$ and compute

$$e^{-\frac{1}{2}ik^2 dt} \mathcal{F}[u(x, t)],$$

where $\mathcal{F}$ denotes the Fourier transform. Then we take the inverse Fourier transform of the expression to find the solution in the physical space, yielding the final expression

$$u(x, t + dt) \sim e^{iN dt} e^{-\frac{1}{2}ik^2 dt} \mathcal{F}^{-1}[u(x, t)].$$

This paper is organized as follows. In Section 2, we discuss the SSFM. Section 3 describes the gPC collocation method. Section 4 contains the gPC collocation algorithm for the NLSE with the singular potential term to detect the critical velocity $V_c$.
Fig. 1. Solution of the linear Schrödinger equation with singular potential. Final time $t = 10$. Top panel: $\epsilon = 0.05$ and the initial position of the soliton $x_0 = 0$ and $x_0 = -20$, respectively. Bottom panel: $\epsilon = 5.0$ and the initial position of the soliton $x_0 = 0$ and $x_0 = -20$, respectively. For each case, the blue solid line represents the real part of the solution and the red dotted line represents the imaginary part of the solution.

We apply SSFM to Eq. (4) where the nonlinear operator $N = |u|^2$ and the linear operator $D$ becomes $L$, $L = \frac{1}{2} \frac{d^2}{dx^2} + \epsilon \delta(x)$. In our numerical simulations we use the high-order SSFM, such as the Strang splitting based on:

$$e^{i dt} N = e^{i dt} L e^{i dt} D + O(dt^3 \left( [L, [L, N]] + [N, [N, L]] \right)).$$

where $[L, N] = LN - NL$ denotes the commutator between $L$ and $N$. Thus, from $t$ to $t + dt$

$$u(x, t + dt) = e^{i dt} N e^{i dt} L e^{i dt} D u(x, t) \approx e^{i dt} L e^{i dt} D u(x, t).$$

(11)

In this calculation, the shape of the $\delta$-function does not matter since as $\int \delta(x) dx = 1$, Eq. (10) becomes

$$u(x, t + dt) = e^{i dt} N e^{i dt} L e^{i dt} D \left[ e^{-\frac{1}{2} dt^2 k^2} u(x, t) + i \epsilon dt \left( u(0, t) e^{-\frac{1}{2} dt^2 k^2} + 3 u(0, t - dt) + u(0, t - 2 dt) \right) \right],$$

which is second order accurate in $t$.

Fig. 1 shows the numerical solution of the linear Schrödinger equation with singular potential:

$$\frac{\partial u}{\partial t} + u_{xx} = -\epsilon \delta(x) u, \quad u(x, 0) = \text{sech}(x - x_0)e^{i V x}.$$

Solution depends on $\epsilon$ but the effect is highly visible when the initial soliton is situated at $x_0 = 0$, the position of the defect. When the initial soliton is far away from the defect, say $x_0 = -20$, the effect of $\epsilon$ is negligible.

3. gPC collocation method

We solve Eq. (4) with the initial condition given by Eq. (7) for both small and large values of $\epsilon$ by the gPC collocation method. We use the gPC method for the solution of the NLSE using the Wiener–Askey scheme [26,28], in which the Hermite,
Legendre, Laguerre, Jacobi and generalized Laguerre orthogonal polynomials are used for modeling the effect of continuous random variables described by the normal, uniform, exponential, beta and gamma probability distribution functions (PDFs), respectively [27]. These orthogonal polynomials are optimal for those PDFs since the weight function in the inner product and its support range correspond to the PDFs for those continuous distributions.

Suppose we have the random variable \( \xi \) and the probability space \( \Gamma = (\Omega, \Sigma, \mathbb{P}) \) equipped with the inner product \( \langle u, v \rangle \), where \( u, v \in L^2(\Gamma) \) and the associated norm \( \| \cdot \|_2 \). \( \mathbb{P} \) is the probability measure. Following the standard gPC expansion, we assume that \( u(x, t, \xi) \) is sufficiently smooth in \( \xi \) and has a converging expansion of the form

\[
    u(x, t, \xi) = \sum_{k=0}^{\infty} \hat{u}_k(x, t) \phi_k(\xi),
\]

where the orthonormal polynomials \( \phi_k(\xi) \) correspond to the PDF of the random variable \( \xi \) and satisfy the following orthogonality relation:

\[
    \mathbb{E}[\phi_k \phi_l] := \int \phi_k(\xi) \phi_l(\xi) \rho(\xi) \, d\xi = \delta_{kl}.
\]

Here \( \delta_{kl} \) is the Kronecker delta and \( \rho(\xi) \) is the weight function. Note that the polynomials are normalized. For example, if the PDF is uniform, \( \rho(\xi) \) is given by

\[
    \rho(\xi) = \frac{1}{2}, \quad \text{for } \xi \in [-1, 1],
\]

and \( \phi_k(\xi) \) is the normalized Legendre polynomial of degree \( k \). The expansion coefficients are given by

\[
    \hat{u}_k(x, t) = \langle u(x, t, \xi), \phi_k(\xi) \rangle.
\]

For the stochastic collocational approach we approximate \( \hat{u}_k(x, t) \) as

\[
    \hat{u}_k(x, t) = \sum_{j=0}^{N} u(x, t, \alpha^j) \phi_k(\alpha^j) \omega^j, \quad k = 0, \ldots, N, \tag{12}
\]

where \( N + 1 \) is the total number of the collocation nodes. Here \( \{\alpha^j, \omega^j\} \) is a set of nodes and weights where \( \alpha^j \in [-1, 1] \), and \( \omega^j \) denote the \( j \)th node and its associated weight, respectively, in the parameter space such that

\[
    \forall f, \exists \tilde{f} \equiv \sum_{j=0}^{N} f(\alpha^j) \omega^j. \tag{13}
\]

Here \( \forall \tilde{f} \) is an approximation of the integral

\[
    \tilde{I}[f] \equiv \int f(p) \rho(p) \, dp = \mathbb{E}[f(p)], \tag{14}
\]

for sufficiently smooth functions \( f \), i.e.,

\[
    \forall \tilde{f} \rightarrow I[f], \quad N \rightarrow \infty.
\]

In this paper we consider \( V \) as the random variable and we choose a collocation nodal set \( \{V^j, \omega^j\}_{j=0}^{N} \), where \( V^j \) are the \( j \)th collocation points and \( \omega^j \) are the corresponding weights. For each \( j = 0, \ldots, N \), we solve the problem given by Eqs. (4) and (7) with the parameters \( \epsilon \) and \( V^j \) and let the solution set be \( \{u_0, \ldots, u_N\} \) where \( u_j \) is the solution for \( V = V^j \). For solving this deterministic equation, we employ the Strang splitting method described above. The approximate gPC expansion coefficients are

\[
    \hat{u}_m(x, t) = \sum_{j=0}^{N} u_j(x, t, V^j) \phi_m(V^j) \omega^j, \quad m = 0, \ldots, N,
\]

where \( \{\phi_m\} \) are the orthonormal polynomials. And finally we construct the \( N \)th order gPC approximation

\[
    u(x, t; V) \approx \sum_{m=0}^{N} \hat{u}_m(x, t) \phi_m(V).
\]
The following algorithm describes how to calculate the critical velocity by using the gPC collocation method.

We use the gPC method to find the critical velocity $V_c$ efficiently for any given $\epsilon$. Here the soliton velocity $V$ is the random variable. Suppose we know in advance that the critical velocity $V_c$ lies between $V_a$ and $V_b$ ($V_a < V_b$) and consider $V$ has a uniform distribution over $[V_a, V_b]$. Let $\xi$ be the map from $V$ to the uniform support $[-1, 1]$ by

$$\xi = \frac{2V - V_a - V_b}{V_b - V_a}.$$}

Since the distribution is uniform, we use the Legendre polynomials for expanding the solution in the random space. Since $V$ itself has the uniform distribution, it is not necessary to have the gPC expansion of $V$. We choose $N + 1$ Gauss–Legendre quadrature points with the weights. Let the set $\{\alpha_i, \omega_i\}_{i=0}^N$ denote the $(N + 1)$ quadrature points $\alpha_i$ and the corresponding weights $\omega_i$.

Now find the solution of Eq. (4) for each $V = \alpha_i$ by using the high-order SSFM. For this purpose one must use a sufficiently large computational domain and sufficiently long time interval. We set up the domain size and the computational final time.

We reconstruct the soliton solution for each simulation for $\hat{u}_i(x, T_f, \alpha_i)$.

Evaluate the approximate gPC expansion coefficients by

$$\hat{u}_m(x, T_f) = \sum_{i=0}^N u_i(x, T_f, \alpha_i) \phi_m(\xi(\alpha_i)) \omega_i,$$

where $\{\phi_m\}_{m=0}^N$ is the set of orthogonal polynomials and $\omega_i$ are the quadrature weights. The full gPC solution is given by

$$u(x, T_f, \alpha) = \sum_{k=0}^N \hat{u}_k(x, T_f) \phi_k(\xi(\alpha)).$$

The mean solution is given by the 1st mode [27], i.e.,

$$\hat{u}_0(x, T_f) = \sum_{i=0}^N u_i(x, T_f, \alpha_i) \phi_0(\xi(\alpha_i)) \omega_i = \sum_{i=0}^N u_i w_i.$$  \hspace{1cm} (16)

**Remark 1.** The solution $u(x, t, V)$ has a jump at $V = V_c$ for $t \to \infty$ because of the critical behavior of the soliton solution around the potential. This means that the spectral reconstruction of $u(x, t, V)$ in $V \in [V_a, V_b]$ using $\hat{u}_l(x, t)$, $l = 0, \ldots, N$ may become oscillatory around $V = V_c$. This was also addressed in our previous work for the critical behavior of the soliton solution of the sine-Gordon equation [6]. Here note that the proposed method in this paper uses only the first moment $\hat{u}_0(x, t)$ to estimate the critical velocity $V_c$ but not the reconstruction of $u(x, t, V)$. The mean solution Eq. (16), $\hat{u}_0(x, t)$ is continuous in the physical space.

The energy of a soliton is defined by $E = \frac{1}{2} \int |u(x, t)|^2 \, dx = A$ [4], where $A$ is the amplitude of the soliton. So the mean of the energy is defined by

$$\bar{E} = \sum_{i=0}^N \omega_i \frac{1}{2} \int |u(x, T_f, \xi(\alpha_i))|^2 \, dx$$

$$= \sum_{i=0}^N \omega_i A$$

$$= A \sum_{i=0}^N \omega_i = A.$$
But in this work, we define the energy with the mean solution, which is different from the mean of the energy, i.e.,

\[
\frac{1}{2} \int_{-L}^{L} |\tilde{u}_0(x, T_f)|^2 \, dx \neq A.
\]

From Eq. (16), we define the average energy \(\tilde{E}_L\) (not the average energy of the whole system) between \([-L, L]\) at the final time \(T_f\), as follows,

\[
\tilde{E}_L = \frac{1}{2} \int_{-L}^{L} |\tilde{u}_0(x, T_f)|^2 \, dx.
\]  

Remark 2. Since the reconstruction of the solution is not used due to the jump at \(V = V_c\), instead of using \(u(x, T_f, \alpha)\) in energy expression, we use \(\tilde{E}_L = \frac{1}{2} \int_{-L}^{L} |\tilde{u}_0(x, T_f)|^2 \, dx\).

Suppose that among \(N\) solutions (for \(N\) quadrature points), \(i\) solutions are trapped inside \([-L, L']\), where \(L' < L\). Since we assume that the distribution of \(V\) over \([V_a, V_b]\) is known and \(V_c \in [V_a, V_b]\) and also soliton preserves its energy [19,4], the value of \(i\) can be estimated for large \(N\) where \(N \to \infty\) by

\[
\frac{i}{N} \approx \frac{V_c - V_a}{V_b - V_a},
\]  

and

\[
\tilde{E}_L \approx \frac{i^2}{N^2},
\]  

where \(V_c\) is the critical velocity for the given value of \(\epsilon\). Thus \(V_c\) is evaluated by

\[
V_c = V_a + (V_b - V_a)\sqrt{\tilde{E}_L}.
\]

For the detailed derivations of Eqs. (18) and (19), please see Appendix A.

We are using the Legendre and Hermite chaos and Eq. (20) holds for high values of \(N\) for these cases. So for the small values of \(N\), this formula does not calculate \(V_c\) accurately. If we increase the number of quadrature points, \(N\), then the critical velocity can be determined more accurately. For our simulations we used 24 Gauss–Legendre quadrature points (\(N = 23\)) and obtained the error accuracy of \(\sim 10^{-12}\). Fig. 8 shows the spectral convergence of the error of the critical velocities with the increasing number of the quadrature points.

In Eq. (20), the convergence of \(V_c\) mainly depends on how \(\tilde{u}_0(x, T_f)\) converges with \(N\). Due to the critical behavior of the solution in the random space, \(u(x, T_f)\) has a jump in terms of \(V\). But the solution \(u(x, T_f)\) is continuous and regular in the physical space for any value of \(V\). Thus the mean solution of \(u(x, T_f)\) over \(V\) is still continuous and regular. Such a smoothness yields the spectral convergence of \(\tilde{u}_0(x, T_f)\). Consequently it is expected that the error of the critical velocity which depends on \(\tilde{u}_0(x, T_f)\) also converges exponentially. In our previous work a similar observation was made [18]. Fig. 8 confirms the spectral convergence of the error in the determination of \(V_c\).

5. Numerical results

We first consider the moderate value of \(\epsilon\), e.g., \(\epsilon = 2.7\). By doing few Monte Carlo simulations we roughly estimate the interval \([V_a, V_b]\) containing \(V_c\). For \(\epsilon = 2.7\), we use \(V_a = 0.1\) and \(V_b = 0.14\). Since for moderate and high values of \(\epsilon\), the simulation time is relatively less than the simulation time with the smaller value of \(\epsilon\), we follow the same procedure to find the suitable intervals. But for the small values of \(\epsilon\), e.g., \(\epsilon < 1.0\), for which the simulation time is long, we use the extrapolation of \(V_c\) from the previous \(\epsilon\) to get the rough estimate of the interval.

Fig. 2 presents the interaction of the soliton with the \(\delta\)-function. Here we choose the initial velocity, \(V_0 = 0\) and the potential strength \(\epsilon = 0.1\). The soliton is located at \(x_0 = -0.3\) initially, which is inside the influence zone of the potential. The nonlinear interaction is observed and the soliton solution exhibits an oscillatory behavior along the line \(x = 0\). This case was discussed in [16,17]. But such an initial condition may not necessarily satisfy the governing equation. The initial position of the soliton must be out of the influence zone of the potential and the soliton must be allowed to move freely before it hits the defect. In all cases we consider the starting point of the soliton, \(x_0\) far from the potential, i.e., outside the influence region of the potential.

Fig. 3 shows the behavior of the soliton solutions in three different cases. If \(\epsilon = 0\), the soliton solution passes unperturbedly. But for nonzero \(\epsilon\), the soliton behavior depends on its initial velocity. For \(\epsilon = 0.1\), the soliton passes through the
Fig. 2. Soliton interactions with the defect with the small value of strength ($\epsilon = 0.1$), where the initial velocity of the soliton is zero. The soliton is trapped and an oscillatory movement is observed.

Fig. 3. Top: Soliton solutions without any defect. Middle: Soliton solutions that pass through the defect with the initial velocity $V = 0.001$ and the defect amplitude $\epsilon = 0.1$. Bottom: Soliton solutions that are trapped by the defect with the initial velocity $V = 0.003$ and the defect amplitude $\epsilon = 0.5$. 
Fig. 4. Top left: Soliton solutions transmitted through the defect when $\epsilon = 0.08$ and $V = 5 \times 10^{-5}$. Top right: Soliton solutions transmitted through the defect when $\epsilon = 0.1$ and $V = 8 \times 10^{-5}$. Bottom left: Soliton solutions trapped by the defect when $\epsilon = 4.5$ and $V = 0.220048$. Bottom right: Soliton solutions transmitted through the defect when $\epsilon = 4.5$ and $V = 0.23995187$. For $\epsilon = 4.5$, the radiation effect is clearly visible.

defect for $V = 0.001$ and for $\epsilon = 0.5$ and $V = 0.003$, soliton is trapped by the defect. For both cases, the soliton passed or trapped as a whole. There is no radiation due to the small soliton velocities [4].

Fig. 4 shows the long time simulations for $(\epsilon, V) = (0.08, 5 \times 10^{-5})$ (top left), $(0.1, 8 \times 10^{-5})$ (top right), $(4.5, 0.220048)$ (bottom left) and $(4.5, 0.23995187)$ (bottom right). For the case that $\epsilon$ is small and $V$ is also small, the soliton propagates without any radiation. But for the high values of $\epsilon$, usually greater than 2.7, where the critical velocity is also high, the radiation effect is observed due to the soliton–defect interaction. The bottom panel of Fig. 4 exhibits the radiation effect for $\epsilon = 4.5$. For both the “trapped” and “transmitted” situations, the radiation effect is observed. The bound state effect is also observed in the bottom right, the details of which were discussed in [15].

Fig. 5 shows the nonlinear interactions of the soliton with different soliton velocities. If the soliton velocity is small, nonlinear property dominates as shown in Fig. 4. During the time of interaction with the defect (the dotted line), the soliton velocity increases and after crossing the defect, the velocity turns into its previous value. When the soliton velocity is high, the linear effect dominates and the soliton velocity does not change during the collision but the direction of the propagation changes. That is, the soliton continues its motion with the same velocity. When a slowly moving soliton hits the defect with high strength ($\epsilon = 4.5$), the soliton is trapped by the defect but due to the nonlinear interactions, radiations and transmissions are also seen (bottom figure).

Fig. 6 shows the mean solutions at $T_f$. This is the first mode of the solution by the gPC collocation method. We used both the Legendre and Hermite chaos. We consider the uniform distribution and normal distribution for the Legendre and Hermite chaos, respectively. The figures in the top panel are obtained using the Legendre chaos for $\epsilon = 0.3$ and 0.5. Those solitons trapped by the defect are confined around the defect. There are multiple peaks in the mean solution, but around $x = 0$ the peaks are higher than the others, which implies that some solitons are trapped, and the rest are transmitted. These figures are used to locate the position of $L'$. The right figure shows the zoomed image of the left figure. As shown in the right figure $L'$ is chosen where the mean solution has the local minimum close to zero in the transmitted region.

For the bottom panel figures in Fig. 6, we plotted the mean solutions and zoomed one for $\epsilon = 2.7, 3.0$ and 4.5. The sharp peaks at $x = 0$ imply that the most of the solutions are trapped in that range of $V$ and some of them are transmitted. We already mentioned that in this region for such a large value of $\epsilon$, the radiation effects are visible, which are also showed in the figure. Several $L'$ are illustrated for different $\epsilon$ in the figure.
Fig. 5. The nonlinear interaction of the soliton with the defect (the dotted line). Top left: The nonlinear interaction is prominent when the soliton hits the defect ($\epsilon = 0.3$) with small velocity ($\sim 10^{-5}$) compared to the interaction with the high velocity ($\sim 10^{-1}$) where $\epsilon = 4.5$ (top right). Bottom: The interaction of slowly moving soliton ($V \sim 10^{-5}$) with the defect with high value of $\epsilon$ ($4.5$).

Next we consider the case that $V$ is normally distributed, for which we use the Hermite polynomials [26] and the Gauss–Hermite quadrature points [14]. Let $V_a = a$, $V_b = b$ and $V \in [a, b]$, $\xi \in [-1, 1]$, $\gamma \in (-\infty, \infty)$. The linear transformation between $V$ and $\xi$ is given by

$$V(\xi) = \left(\frac{b - a}{2}\right)\xi + \frac{1}{2}(a + b)$$

and the transformation between $\xi$ and $\gamma$ is given by [7]

$$\gamma = \frac{\xi}{1 - \xi^2}, \quad \xi \neq 0,$$

$$0 \quad \xi = 0.$$  

We have

$$\xi = -1 + \frac{\sqrt{1 + 4\gamma^2}}{2\gamma}, \quad \gamma \neq 0,$$

$$0 \quad \gamma = 0.$$
Fig. 6. The first mode (mean) of the gPC expansion for different $\epsilon$. Top and middle: The Legendre chaos. Bottom: The Hermite chaos. Right figures of the top and middle panels show the locations of $L'$ for different $\epsilon$.

Thus we have

$$ V(\gamma) = \left( \frac{b-a}{2} \right) \left[ -1 + \sqrt{1 + 4\gamma^2} \right] + \frac{1}{2} (a+b), $$

where $\gamma$ has the normal distribution with mean 0 and the standard deviation (SD) 0.1. For the simulation we consider $\epsilon = 0.3$ and $V \sim N(0,0.1)$. The last figure in Fig. 6 shows the mean solution at the final time obtained by the Hermite chaos. Although the mean solutions obtained from the Legendre and Hermite chaos are different, we observe that the location of $L'$ is same for both cases.

Using a series of those simulations above for different values of $\epsilon$, $\epsilon \in [0.05, 4.5]$, we determine the critical velocities. The results are plotted in semi-logarithmic scale in Fig. 7. It is observed that for the small values of $\epsilon$ where $\epsilon < 0.1$, the curve is very stiff and the slope changes sharply around $\epsilon = 0.1$. From $\epsilon > 0.1$, the curve increases steadily. The "trapped" and the "untrapped" regions are clearly shown in the figure. The $V-\epsilon$ graph is the boundary of those two regions.

In order to check the convergence we define the error of the critical velocities by

$$ \text{Error}^\epsilon(N_2) = |V_c^\epsilon(N_2) - V_c^\epsilon(N_1)|, \text{ where } N_2 > N_1 $$
Fig. 7. The critical velocity vs. $\epsilon$ where $\epsilon \in [0.05, 4.5]$.

Fig. 8. Spectral convergence of the critical velocities for $\epsilon = 0.3, 1.0$ and 4.5. The graph shows the spectral convergence for both the Legendre and Hermite chaos. Note that the Legendre chaos shows faster convergence than the Hermite chaos.

where $N_i$ is the number of collocation points. Fig. 8 shows the convergence of errors obtained by the Legendre and Hermite chaos. We do the convergence analysis for various values of $\epsilon$. We choose $\epsilon = 0.3$ (small), $\epsilon = 1.0$ (moderate) and $\epsilon = 4.5$ (high). For the Legendre chaos, the critical velocities for different $N$ are presented in Table 1. For $\epsilon = 0.3$ and $\epsilon = 1.0$, we calculate the errors for both the Legendre and Hermite chaos and for $\epsilon = 4.5$ we use the Legendre chaos. For the Hermite chaos, we expect to have the similar results. The graphs are plotted in semi-logarithmic scale. Fig. 8 confirms spectral convergence but the convergence rates are different for different cases. For $\epsilon = 0.3$ and $\epsilon = 1.0$, the Hermite chaos exhibits slower convergence rate than the Legendre chaos. Also the convergence rate decreases with $\epsilon$. That is, the smaller is the value of $\epsilon$, the faster convergence is obtained. One of the possible reasons is because of the radiation effect. As $\epsilon$ increases, the radiation effect becomes prominent and it affects the convergence of $\hat{u}_0(x, T_f)$. In summary: The numerical scheme stated in Section 4 to find the critical velocity $V_c$ yields spectral convergence and the rate of convergence decreases with $\epsilon$. 

Table 1
Convergence of \( V_c \) with \( N \) for the Legendre chaos. \( \epsilon = 0.3, 1.0 \) and 4.5.

| \( N \) | \( V_c \times 10^3 \) |
|---|---|
| \( \epsilon = 0.3 \) | \( \epsilon = 1.0 \) | \( \epsilon = 4.5 \) |
| 2 | 1.14371292515371 | 19.84534567231890 | 227.14634567231890 |
| 4 | 2.373296704309538 | 21.84060798728778 | 250.050221999967 |
| 8 | 2.417965063524635 | 21.92973308110116 | 253.5223907045220 |
| 12 | 2.419549956717096 | 21.93371415280669 | 254.0471981647718 |
| 16 | 2.419606190849615 | 21.93389198074770 | 254.1266309882442 |
| 20 | 2.419608186111930 | 21.93389992403004 | 254.1386533334490 |
| 24 | 2.419608256906508 | 21.93390027884343 | 254.1404733334490 |

6. Conclusion

In this work we proposed an efficient method of determining the critical soliton velocities, \( V_c \), by using the gPC collocation method. We studied the wide range of \( \epsilon \), i.e., \( \epsilon \in [0.05, 4.5] \). For \( \epsilon < 0.05 \) the numerical simulation demands a huge computational time due to the very small value of the soliton velocity \( (V \sim 10^{-8}) \). We also showed the convergence analysis to prove the merit of our proposed numerical scheme. We found the spectral convergence in all cases. The main development of this paper is the use of the gPC collocation method to determine the critical velocity of the soliton for given \( \epsilon \) with the desired level of accuracy. This is the first paper that uses gPC to find the critical parameter value of NLSE. We obtained \( V_c \) accurately with a small number of simulations. In our future work, we will further study the case that \( \epsilon \ll 0.05 \). Also of high value of \( \epsilon \), where radiation effect is prominent and the convergence of the proposed method becomes slower due to the radiation effect, an efficient numerical method dealing with this effect will be investigated.

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Appendix A

In Eq. (18), we have claimed
\[
i \frac{i}{N} \approx \frac{V_c - V_a}{V_b - V_a}, \quad \text{as } N \to \infty.
\]

For the general and arbitrary distributions, the equation may not hold but it holds for the Legendre and Hermite chaos that we consider in this paper. For the Legendre chaos, where the uniform distribution is used, the points are equally spaced between \( V_a \) and \( V_b \). Thus Eq. (18) satisfies exactly. But for the Hermite chaos, the points are not equally spaced. We denote \((x_i(N))\) or \((x_i)\), the zeros of the Hermite polynomial of degree \( N \) as defined in the paper.

Let
\[
h_i = V(x_{i+1}) - V(x_i).
\]

Then by Eq. (21),
\[
h_i = \frac{V_b - V_a}{2} \left[ -\frac{1 + \sqrt{1 + 4x_i^2}}{2x_{i+1}} - \frac{1 - \sqrt{1 + 4x_i^2}}{2x_i} \right]. \tag{22}
\]

We will show, for large \( N \), \( h_{i+1}/h_i \approx 1 \). We have
\[
\sqrt{1 + 4x_i^2} = 2x_i \left( 1 + \frac{1}{8x_i^2} + O \left( \frac{1}{x_i^4} \right) \right)
= 2x_i + \frac{1}{4x_i} + O \left( \frac{1}{x_i^3} \right). \tag{23}
\]

Eqs. (22) and (23) lead to
\[
\frac{h_{i+1}}{h_i} = \frac{1 - \frac{x_{i+1}}{x_i} + \frac{x_{i+1}}{4x_{i+2}} - \frac{1}{4x_{i+1}} + O \left( \frac{1}{x_i^4} \right)}{\frac{x_{i+2} - x_{i+1}}{x_i} - 1 + \frac{x_{i+1}}{4x_{i+2}} + O \left( \frac{1}{x_i^4} \right)}
= \frac{x_{i+2} - x_{i+1} - 1}{x_{i+1} - x_i} \frac{x_i}{x_{i+2}} \left[ 1 + O \left( \frac{1}{x_i^3} \right) \right]. \tag{24}
\]
Now according to Elbert and Muldoon [10],

\[ x_i = \Lambda - a^i \Lambda^{-\frac{3}{2}} + O(\Lambda^{-\frac{5}{2}}), \quad \text{with} \quad \Lambda = \sqrt{2N + 1}. \]

So we have

\[
\frac{x_i}{x_{i+2}} = 1 + (a^{(i+2)} - a^{(i)})\Lambda^{-\frac{3}{2}} + O(\Lambda^{-\frac{5}{2}}),
\]

\[
\frac{x_{i+2} - x_{i+1}}{x_{i+1} - x_i} = \frac{(a^{(i+1)} - a^{(i+2)})\Lambda^{-\frac{3}{2}} + O(\Lambda^{-\frac{5}{2}})}{(a^{(i)} - a^{(i+1)})\Lambda^{-\frac{3}{2}} + O(\Lambda^{-\frac{5}{2}})},
\]

where \( a^{(i)} \) is the \( i \)th positive root of:

\[
Ai(-x) \cos N - Bi(-x) \sin N = 0,
\]

where \( Ai, Bi \) are the Airy functions [2].

Now for \( x \) large

\[
Ai(-x) \sim \frac{\sin\left(\frac{2x^\frac{3}{2}}{\sqrt{\pi}} + \frac{\pi}{4}\right)}{\sqrt{\pi x^\frac{1}{2}}}, \quad Bi(-x) \sim \frac{\cos\left(\frac{2x^\frac{3}{2}}{\sqrt{\pi}} + \frac{\pi}{4}\right)}{\sqrt{\pi x^\frac{1}{2}}}. \tag{28}
\]

From Eq. (27),

\[
\frac{Ai(-x)}{Bi(-x)} = \tan N. \tag{29}
\]

From Eq. (28),

\[
\frac{Ai(-x)}{Bi(-x)} \sim \tan\left(\frac{2x^\frac{3}{2}}{3} + \frac{\pi}{4}\right). \tag{30}
\]

So from Eqs. (27)–(30),

\[
a^{(i)} \sim \left[\frac{3}{2} \left( N + i\pi - \frac{\pi}{4}\right)\right]^\frac{2}{3} = \left(\frac{3N}{2}\right)^\frac{3}{2} \left[1 + \frac{2\pi i}{3N} - \frac{\pi}{6N} O(N^{-2})\right]. \tag{31}
\]

From Eqs. (24)–(31), we have

\[
\frac{h_{i+1}}{h_i} = \left[1 + (a^{(i+1)} - a^{(i)})\Lambda^{-\frac{3}{2}} + O(\Lambda^{-\frac{5}{2}})\right]^{-\left[-\frac{3N}{2} - \frac{\pi}{2} + O(N^{-\frac{5}{2}})\right] \Lambda^{-\frac{3}{2}} + O(\Lambda^{-\frac{5}{2}})}
\]

\[
\sim 1 \quad \text{as} \quad N \to +\infty. \tag{32}
\]

Thus the claim is established.

In Eq. (19), we claim

\[
\tilde{E}_i \approx \frac{t^2}{N^2},
\]

where

\[
\tilde{E}_i = \frac{1}{2} \int_{-L}^{L} |\tilde{u}_0(x, T_f)|^2 \, dx
\]

with

\[
\tilde{u}_0(x, T_f) = \frac{1}{N} \sum_{k=1}^{N} u_k(x, T_f).
\]

We know,
\[ \frac{1}{2} \int_{-L}^{L} \left| \tilde{\phi}_0(x, T_f) \right|^2 \, dx = \frac{1}{2N^2} \sum_{k,l=1}^{N} \int_{-L}^{L} (u_k \tilde{u}_l)(x, T_f) \, dx \]

\[ = \frac{1}{2N^2} \sum_{k=1}^{N} \int_{-L}^{L} |u_k|^2(x, T_f) \, dx + \frac{1}{2N^2} \sum_{k=1, k \neq \ell}^{N} \int_{-L}^{L} (u_k \tilde{u}_\ell)(x, T_f) \, dx \]

\[ + \frac{1}{2N^2} \sum_{k=1}^{N} \sum_{\ell=1}^{N} \sum_{l=1, l \neq k}^{N} \int_{-L}^{L} (u_k \tilde{u}_l)(x, T_f) \, dx, \]

where \((u_k)_{k \leq 1}\) are trapped by the defect.

Now \(\forall \epsilon > 0, \exists L\) (sufficiently large) for which \(k, l \in \{i+1, \ldots, N\}; \ k \neq l\) and

\[ \left| \int_{-L}^{L} (u_k \tilde{u}_l)(x, T_f) \, dx \right| < \epsilon. \]

Also \(\forall \epsilon > 0, \exists L\) (sufficiently large) for which \(k \in \{1, \ldots, i\}, l \in \{i+1, \ldots, N\}\) and

\[ \left| \int_{-L}^{L} (u_k \tilde{u}_l)(x, T_f) \, dx \right| < \epsilon. \]

Now setting \(A := \frac{1}{2} \int_{-L}^{L} |u_k(x, T_f)|^2 \, dx\), we get

\[ \left| \frac{1}{2} \int_{-L}^{L} |\tilde{\phi}_0(x, T_f)|^2 \, dx - \frac{A}{N} - \frac{i(i - 1)}{N^2} \right| < \frac{1}{2N^2} \left(N^2 - i^2 - N + i + 1 \right) < \epsilon. \]

Now for \(N\) and \(i\) large enough, we also have, \(\frac{A}{N} < \epsilon\) and \(\frac{i(i - 1)}{N^2} < \epsilon\), so that

\[ \left| \frac{1}{2} \int_{-L}^{L} |\tilde{\phi}_0(x, T_f)|^2 - \frac{i^2}{N^2} A \right| < 3\epsilon \]

(\(\epsilon\) as small as wanted). In this paper, \(A = 1\). Thus

\[ \frac{\epsilon}{N^2} \approx \frac{i^2}{N^2}, \]

holds for large \(N\).

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