Accuracy of an approximate variational solution procedure for the nonlinear Schrödinger equation

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An assessment is made of the accuracy of a direct variational method for obtaining approximate analytical solutions of the nonlinear Schrödinger equation. The method involves trial functions and a Rayleigh-Ritz optimization procedure. The accuracy of the approximation scheme is inferred from the ability of the optimized solution to preserve the invariants of the nonlinear Schrödinger equation.

Nonlinear pulse propagation in optical fibers can be modeled by the nonlinear Schrödinger (NLS) equation and extensions of this equation. Although the NLS equation can be solved exactly using the inverse scattering theory,¹ the corresponding solutions are not very explicit except for the simplest soliton solutions. A major contribution to the understanding of the properties of the NLS equation and related equations has come from numerical investigations.²⁻⁴ However, numerical investigations do not give the same summarized information and physical insight as an explicit analytical solution. This situation emphasizes the need for approximate analytical solutions and several such methods have been suggested using, for example, the invariants of the NLS equation,⁵ moment method,⁶ and a variational method based on a Rayleigh-Ritz optimization procedure.⁷

In particular, the variational method has proven to be a flexible and powerful tool for investigating the dynamic behavior of optical pulses under a variety of physical situations. However, the application of the variational Rayleigh-Ritz optimization procedure involves a trialfunction ansatz to model the evolution of the pulse. Since the result depends crucially on the choice of trial functions, the application of the method to a specific problem requires physical intuition and a fair amount of qualified guessing. Furthermore, in order to arrive at analytical explicit results, a compromise has to be made between two contradictory requirements: the trial function has to be flexible, i.e., complicated enough to describe the main characteristics of the exact solution, but still simple enough to make the subsequent algebra feasible.

The accuracy of an approximate variational solution is mostly tested by comparison with the results of numerical investigations or with exact analytical solutions available in certain limits. However, an inherent problem associated with variational methods based on the analytical Rayleigh-Ritz optimization procedure in Ref. 7 is to assess *a priori* the accuracy of the optimized solution.

In the present work we will demonstrate that important information on the accuracy of the variational solution can be inferred from an investigation of the extent to which the optimized trial function preserves the invariants of the NLS equation. In this respect the analytical approach is similar to numerical solution procedures, which at suitable steps evaluate the energy invariant to check the numerical accuracy. The present analysis shows that in parameter regions where the relative errors in the higher-order invariants are small, the variational solution indeed gives a good description of the exact solution. Conversely, large relative errors in the invariants signal that the accuracy of the solution deteriorates. These results make it possible to *a priori* assess the qualitative accuracy of a variational approximation.

The nonlinear Schrödinger equation, which determines the evolution of the slowly varying envelope function $\Psi(x,\tau)$ of an optical pulse can be written¹⁻⁷

$$i\frac{\partial\Psi}{\partial x} = \alpha \frac{\partial^2\Psi}{\partial\tau^2} + \kappa |\Psi|^2 \Psi , \qquad (1)$$

where x denotes distance of propagation, τ denotes retarded time, and α and κ characterize dispersion and nonlinearity, respectively. In the variational approach, Eq. (1) is reformulated as a variational problem, viz.,

$$\delta \int_0^\infty \int_{-\infty}^\infty \left[\frac{i}{2} \left[\Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x} \right] - \alpha \left| \frac{\partial \Psi}{\partial \tau} \right|^2 + \frac{\kappa}{2} |\Psi|^4 \right] d\tau \, dx = 0 \; . \tag{2}$$

Consider, for example, the evolution of an initially Gaussian-shaped pulse, i.e.,

$$\Psi(0,\tau) = A_0 \exp(-\tau^2/2a_0^2) . \tag{3}$$

Physical intuition based on well-known results from linear and nonlinear pulse propagation theory predicts that, in order to model the subsequent evolution of the pulse, an ansatz function must be used which is flexible enough to allow changes in pulse width and pulse amplitude, as well as the development of a frequency chirp. A natural choice of trial function which incorporates these features is

$$\Psi(x,\tau) = A(x) \exp\{\left[-\frac{\tau^2}{2a^2(x)}\right] + ib(x)\tau^2\}, \quad (4)$$

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where $A(0) = A_0$, $a(0) = a_0$, and b(0) = 0. Note that, whereas the pulse amplitude, width, and chirp factor are undetermined functions of x, the functional dependence on τ is prescribed; the pulse is assumed to remain Gaussian in shape and the chirp frequency is assumed to vary linearly with τ . This fact makes it possible to perform the τ integration in the functional (2) and to reduce the variational problem to the following form:

$$\delta \int_{0}^{\infty} \frac{\sqrt{\pi}}{2} \left[ia \left[A \frac{dA^{*}}{dx} - A^{*} \frac{dA}{dx} \right] + |A|^{2} a^{3} \frac{db}{dx} - \alpha a^{3} |A|^{2} \left[4b^{2} + \frac{1}{a^{4}} \right] + \frac{1}{\sqrt{2}} \kappa a |A|^{4} \right] dx = 0 .$$
 (5)

The Euler-Lagrange equations corresponding to Eq. (5) become a system of coupled nonlinear ordinary differential equations:

$$\frac{\partial \langle L \rangle}{\partial y_i} - \frac{d}{dx} \frac{\partial \langle L \rangle}{\partial (dy_i/dx)} = 0, \text{ where } y_i = A, A^*, a, b$$
(6)

and $\langle L \rangle$ denotes the integrand of Eq. (5). This system of equations can be reduced to three equations expressing A, A^* , and b in terms of a, plus a single equation for a. The second-order nonlinear equation for a can be integrated once and cast into a physically suggestive form,

viz., that of a particle moving in a potential well:

$$\frac{1}{2} \left[\frac{da}{dx} \right]^2 + \Pi(a) = 0 , \qquad (7)$$

where the potential $\Pi(a)$ is given by

$$\Pi(a) = 2\alpha^2 \left[\frac{1}{a^2} - \frac{1}{a_0^2} \right] - \alpha \kappa a_0 |A_0|^2 \sqrt{2} \left[\frac{1}{a} - \frac{1}{a_0} \right] .$$
(8)

The variation of the pulse width with distance may be monotonic or oscillatory, depending on the form of $\Pi(a)$, which is determined by the value of the characteristic parameter

$$\xi = -\kappa |A_0|^2 a_0^2 / \alpha \sqrt{2} . \tag{9}$$

The parameter ξ depends on the pulse parameters as well as on the ratio of the dispersion to the nonlinearity of the optical fiber. Nonlinear effects will enhance or counteract the ordinary linear dispersive pulse spreading, depending on whether $\xi > 0$ or $\xi < 0$, respectively. If $-1 < \xi < 0$, nonlinear compression effects are too weak to balance the spreading and the pulse width increases monotonically, although less rapidly than in the linear case. Thus for $\xi > -1$ the following solution is obtained for the normalized pulse width $y(x) = a(x)/a_0$:

$$x\frac{2|\alpha|}{a_0^2} = \frac{\{(y-1)[y+1/(1+\xi)]\}^{1/2}}{\sqrt{1+\xi}} + \frac{\xi(1+\xi)^{-3/2}}{2}\ln\frac{2(1+\xi)(y+\{(y-1)[y+1/(1+\xi)]\}^{1/2}) - \xi}{2+\xi} .$$
 (10)

For $-2 < \xi < -1$, the pulse initially broadens but the nonlinear compression effect is strong enough to stop the pulse broadening and to give rise to an oscillatory behavior. For $\xi < -2$, the nonlinearity becomes so strong that the pulse initially compresses until linear dispersion stops the compression and again an oscillatory behavior results. The corresponding solution of Eq. (7) is given by

$$x\frac{2|\alpha|}{a_0^2} = \frac{-\operatorname{sgn}(2+\xi)}{\left[-(1+\xi)\right]^{1/2}} \left[(1-y)\left[y+\frac{1}{1+\xi}\right] \right]^{1/2} + \frac{\xi}{2\left[-(1+\xi)\right]^{3/2}} \left[\pm \left[\operatorname{arcsin}\frac{2(1+\xi)y-\xi}{2+\xi}-\frac{\pi}{2}\right] + k2\pi \right].$$
(11)

For a detailed discussion of the properties of Eq. (7) and the corresponding solutions, see Ref. 7. In the present context it is sufficient to emphasize the following points: (i) When $\xi = 0$, i.e., in the linear case, the variational solution reduces to the well-known spreading Gaussian. Thus, in this case, the variational solution coincides with the exact solution of the problem. This is possible since the exact solution is within the set of trial functions. (ii) When $\xi = -2$, the variational solution yields a Gaussian pulse with constant parameters. This Gaussian pulse provides a good approximation of the correct soliton solution, cf. Ref. 7. On the other hand, if sech-shaped pulses had been used as trial functions, the exact soliton would have been obtained, whereas the variational solution of the linear problem would have been a sech approximation of the spreading Gaussian. (iii) For large negative values of ξ , the solution enters the parameter region of higher-order solitons, which involve pulse splitting and very complex amplitude variation. Although the approximate variational solution still contains features that are in qualitative agreement with the exact solution, cf. Ref. 7, the trial function is not flexible enough to model the pulse splitting behavior and the quantitative accuracy of the approximate solution deteriorates.

The general accuracy of the variational solution was assessed in Ref. 7 by comparison with exact results from inverse scattering theory and results obtained by numerical investigations of the NLS equation. In the present work we will present a new approach which yields *a priori* information on the accuracy of the approximate variational solution. The approach should be equally useful for other nonlinear evolution equations.

It is well known that the NLS equation has an infinite

number of invariants,¹ of which the first five read

$$I_1 = \int_{-\infty}^{\infty} |\Psi|^2 d\tau , \qquad (12a)$$

$$I_2 = \int_{-\infty}^{\infty} \left[\Psi \frac{\partial \Psi^*}{\partial \tau} - \Psi^* \frac{\partial \Psi}{\partial \tau} \right] d\tau , \qquad (12b)$$

$$I_{3} = \int_{-\infty}^{\infty} \left[\alpha \left| \frac{\partial \Psi}{\partial \tau} \right|^{2} - \frac{\kappa}{2} |\Psi|^{4} \right] d\tau , \qquad (12c)$$

$$I_4 = \int_{-\infty}^{\infty} \left[\alpha \Psi \frac{\partial^3 \Psi^*}{\partial \tau^3} + \frac{3\kappa}{2} \Psi |\Psi|^2 \frac{\partial \Psi^*}{\partial \tau} \right] d\tau , \qquad (12d)$$

$$I_{5} = \int_{-\infty}^{\infty} \left[\alpha^{2} \left| \frac{\partial^{2} \Psi}{\partial \tau^{2}} \right|^{2} + \frac{\kappa^{2}}{2} |\Psi|^{6} - \frac{\alpha \kappa}{2} \left[\frac{\partial}{\partial \tau} |\Psi|^{2} \right]^{2} - 3\alpha \kappa \left| \frac{\partial \Psi}{\partial \tau} \right|^{2} |\Psi|^{2} \right] d\tau . \qquad (12e)$$

The information contained in the (infinite) set of invariants is equivalent to that of the original NLS equation. The lower-order invariants have direct physical significance, e.g., the first invariant expresses conservation of pulse energy. Higher-order invariants involve higher-order derivatives, more complicated interplay between nonlinear and dispersive effects, and more detailed information about the fine structure of the pulse. Intuitively we expect that if an approximate solution is inserted into the functionals defining the invariants, important information on the accuracy of the approximation is provided by the number of functionals that remain invariant and the relative error of the nonconserved functionals.

If we use our approximate variational solution to calculate the first five invariants, Eq. (12), we find

$$I_1 = \sqrt{\pi} a_0 |A_0|^2 = \text{const}$$
, (13a)

$$I_2 = 0 = \text{const} , \qquad (13b)$$

$$I_{3} = \frac{\sqrt{\pi}}{2} |A_{0}|^{2} \left[\frac{\alpha}{a_{0}} - \frac{\kappa a_{0} |A_{0}|^{2}}{\sqrt{2}} \right] = \text{const}, \quad (13c)$$

$$I_4 = 0 = \text{const} , \qquad (13d)$$

$$I_{5} = \mu a_{0} |A_{0}|^{2} \sqrt{\pi} \left[\frac{3}{8} (1+\xi)^{2} - \frac{3}{8} \xi (1+\xi) \frac{1}{y(x)} + \frac{\xi^{2}}{2\sqrt{3}} \frac{1}{[y(x)]^{2}} + \frac{\xi}{4} \frac{1}{[y(x)]^{3}} \right].$$
(13e)

We notice that the first four invariants are indeed preserved, although I_2 and I_4 vanish simply because an initially symmetric pulse will remain symmetric during propagation. The conservation of pulse energy, as expressed by the invariant I_1 , is a common feature in many evolution equations. However, the third invariant I_3 is more closely related to the NLS equation and its corresponding Lagrangian, cf. Eq. (2), by being the first invariant to include the nonlinearity. The conservation of I_3



FIG. 1. The normalized fifth invariant as a function of distance of propagation for $\xi = -3$ and 4, respectively.



FIG. 2. The asymptotic normalized value of the fifth invariant $\lim_{x\to\infty} I_5(x)/I_5(0)$ as a function of ξ .



FIG. 3. Contour plot of the normalized fifth invariant, i.e., $I_5(y,\xi)/I_5(1,\xi) = \text{const.}$

expresses the well-known property that the Hamiltonian is a constant of motion in cases where the Lagrangian does not depend explicitly on the coordinate of evolution. The fact that the approximate variational solution preserves the four first invariants and, in particular, I_3 , indicates that it should be able to describe the main characteristics of the interaction between dispersive and nonlinear effects in the NLS equation. Furthermore, this explains the fact that the invariant method and the variational method give the same prediction for the pulse width variation, cf. Ref. 5.

The fifth invariant is not conserved except for two cases: $\xi = -2$ and 0, i.e., the soliton case and the purely linear case for which the variational solution is indeed a good approximation of the exact solution. In all other cases, I_5 will depend on x. For $\xi > -1$, $I_5(x)$ will tend towards an asymptotic value whereas for $\xi < -1$, $I_5(x)$ will vary periodically. Figure 1 illustrates the variation of $I_5(x)/I_5(0)$ for $\xi = -3$ and 4, respectively, and Fig. 2 shows the asymptotic value $\lim_{x\to\infty} I_5(x)/I_5(0)$ as a function of $I_5(x)/I_5(0)=$ const in the (y,ξ) plane. Figures 1–3 together indicate that in certain parts of parameters.

eter space, the relative error in the fifth invariant becomes large, which indicates that the variational solution is not a good approximation. The regions around $\xi = -1$ and $\xi < -4$ are particularly bad, cf. Fig. 3. At $\xi = -1$ the approximate solution changes character from bound (soliton) oscillatory solutions to monotonic dispersive pulse spreading. The trial functions are not flexible enough to describe the splitting of the pulse into a soliton part and a significant dispersively decaying shed off pulse, and the accuracy deteriorates. For large negative ξ $(\xi < -4)$, higher-order solitons form, which involve too complicated amplitude variations, e.g., pulse splitting, to be modeled by a simple pulse ansatz. Again the accuracy deteriorates. Away from these regions the relative "error" in the fifth invariant is small, indicating that the optimized trial function is a good approximation of the exact solution.

Thus we conclude that the qualative accuracy of an approximate solution of a nonlinear evolution equation can be inferred from an evaluation of the errors in the invariants associated with the equation. The advantage of this approach is the fact that it is an *a priori* assessment; no comparisons with numerical results are necessary.

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