Unexpected behavior of nonlinear Schrödinger solitons in an external potential

Helge Frauenkron and Peter Grassberger
Physics Department, University of Wuppertal, D-42097 Wuppertal, Germany

(Received 5 September 1995)

Employing a higher order symplectic integration algorithm, we integrate the one-dimensional nonlinear Schrödinger equation numerically for solitons moving in an external potential. In particular, we study the scattering off an interface separating two regions of constant potential, with a linearly rising ramp in the interface region. Transmission coefficients are computed as functions of the height of this ramp and of its steepness in the semiclassical domain (slope $\ll 1$) near the classical threshold for transmission. For energies slightly above this threshold, we find a narrow range of slopes in which the soliton is almost fully reflected, though it is nearly completely transmitted outside this range.

PACS number(s): 03.40.Kf, 03.65.Ge, 42.81.Dp

Recent years have seen a considerable growth in the interest in nonlinear partial differential equations with soliton solutions. In particular, the nonlinear Schrödinger equation (NLSE) and its modifications have a quite large range of applicability, describing phenomena occurring in optics, solid state, particle, and plasma physics. Some of the more interesting problems, for which the NLSE appears to provide a fruitful description, are modulational instability of water waves [1], propagation of heat pulses in anharmonic crystals, helical motion of very thin vortex filaments, nonlinear modulation of collisionless plasma waves [2], and self-trapping of light beams in optically nonlinear media [3–5]. In all these problems, the main interest lies in the fact that the NLSE has soliton solutions. These are solitary waves with well-defined pulse-like shapes and remarkable stability properties [6].

A great deal of current interest is directed to the influence of external perturbations on these states. Such perturbations can be due to different sources. One interesting class consists of "Hamiltonian" perturbations that do not destroy the Hamiltonian structure of the NLSE. There are essentially two kinds, one arising from the interaction with a potential term, the other due to spatial inhomogeneity of the coefficients in the kinetic and nonlinear terms. The latter [4,5,7–9] are relevant for the transmission of pulses through junctions in optical fibers.

In this paper we will limit ourselves to external potentials that are constant outside a finite interval. But we allow different values V_0 for $x \to \pm\infty$, modeling thereby an interface between two different media. This interface can have different widths, which can be described by a linearly rising potential with adjustable slope. We study initial conditions consisting of a single soliton moving with constant velocity. In general, we have to expect that this soliton will have a complicated interaction when it hits the interface. It can be reflected, break up into several solitons, radiate nonsolitary waves, or can show any combination of these.

Several authors [3–5,10,11] have studied this problem by means of perturbation theory. But the perturbations examined there are much smaller than those that will be discussed in the present paper. Therefore their approach will not necessarily hold in the present case. An exception is provided by the semiclassical limit, where the potential varies slowly on length scales given by the size of the soliton. In this limit (corresponding to the slope in the interface tending to 0), we have Ehrenfest's theorem, which tells us that the soliton behaves like a classical particle: it is transmitted without radiating nonsolitary waves if the potential height is below some threshold, while it is totally reflected above.

It seems natural to assume—and was assumed in all previous works—that the approach to this semiclassical limit is smooth. Thus, there should exist a semiclassical regime where the transmission coefficient depends essentially only on the potential difference, but is weakly dependent on the slope, provided it is sufficiently small. It is the purpose of the present paper to show that this is *not* the case. Assume that the kinetic energy K of the soliton is such that it could just barely overcome the potential classically, $K = V_0 + \epsilon$. We find that there is for any sufficiently small ϵ a sharply defined range in slopes—extending to zero slope in the limit $\epsilon \to 0$—where the soliton is nearly completely reflected. This is so in spite of the fact that it would be transmitted classically, as it does indeed outside this range. This phenomenon could have a number of interesting practical applications.

For the numerical integration of the NLSE we applied a fourth-order symplectic integrator. As we have already mentioned, the NLSE is a Hamiltonian system. Thus, it is natural to apply to it integration routines that were developed during the recent years and whose main characteristic is that they preserve the Hamiltonian structure [12–14]. These symplectic integrators were successfully applied to the linear [15–18] and nonlinear [19–23] Schrödinger equations. For this reason we will not go into further discussion and refer the reader to the existing literature.

One very important advantage of these kinds of integrators with respect to the most common ones, such as, e.g., Runge-Kutta or predictor-corrector, is that the energy might fluctuate, but does not drift. This, together with the fact that normalization is exactly preserved for these integrators, implies that they have extremely good long-time stability.

Using appropriate units, we can write the NLSE as

$$i\frac{\partial\Psi(x,t)}{\partial t}=-\frac{1}{2}\frac{\partial^2\Psi(x,t)}{\partial x^2}-|\Psi(x,t)|^2\Psi(x,t)+V(x)\Psi(x,t)\ , \tag{1}$$

where $V(x)$ is the external potential. We will use for the latter a piecewise linear ansatz, with $V(x)\equiv 0$ for $x<0$, $V(x)\equiv V_0>0$ for $x>x_0\geq 0$, and a linearly rising ramp for x between 0 and x_0,

$$V(x)=\begin{cases}0\ , & x<0\\ xV_0/x_0\ , & 0\leq x<x_0\\ V_0\ , & x\geq x_0\ .\end{cases} \tag{2}$$

We call the negative x-axis region I, while region II is the region $x>0$.

We study scattering solutions where the incoming wave consists of a single soliton arriving from region I. The outgoing wave will then in general be a complicated superposition of solitons and nonsolitary waves. One interesting question is how much of the total energy is transmitted and reflected. For a constant potential V_0 the soliton solutions of Eq. (1) form a two-parameter manifold (apart from translations). Taking as parameters the velocity v and the amplitude a, these solutions read [24]

$$\Psi(x,t)=\frac{a}{\cosh[a(x-vt)]}e^{i\{vx+[(a^2-v^2)/2-V_0]t\}}\ . \tag{3}$$

We denote the velocity of the incoming soliton as v_0. Using a suitable rescaling of x, t, and Ψ, we can always choose its amplitude as $a_0=\frac{1}{2}$, without loss of generality.

Among the infinitely many conserved quantities [for $V(x)=\text{const.}$] the following two are of particular interest: the normalization,

$$N=\int|\Psi|^2dx \tag{4}$$

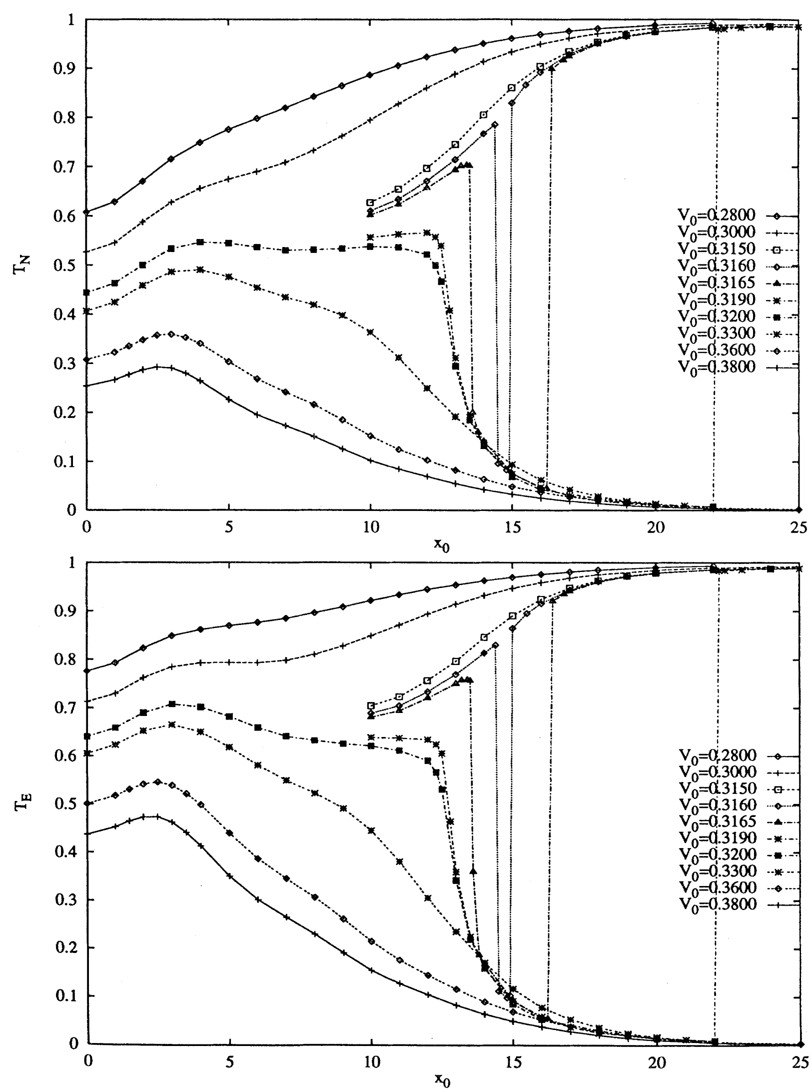

FIG. 1. The transmission coefficients T_N and T_E vs x_0 for different potential heights.

and the energy

$$E=\int\left[\frac{1}{2}\left|\frac{\partial\Psi}{\partial x}\right|^2-\frac{1}{2}|\Psi|^4+V(x)|\Psi|^2\right]dx\ . \tag{5}$$

For the soliton given by Eq. (3) this yields $N=2a$ and $E=(v^2/2-a^2/6)N+\langle V\rangle N$, where the average over $V(x)$ is taken with weight $\propto|\Psi|^2$ as indicated by Eq. (5). Moreover, it is easily seen that N and E are also conserved for nonconstant potential V.

Thus we can define two sets of transmission and reflection coefficients

$$T_N=N_{\rm II}/N\ ,\quad T_E=E_{\rm II}/E \tag{6}$$

and

$$R_N=N_{\rm I}/N=1-T_N\ ,\quad R_E=E_{\rm I}/E=1-T_E\ . \tag{7}$$

For the simulations we used the fourth-order symplectic integrator introduced by McLachlan and Atela [25]. Its application to the NLSE uses a spatial discretization and is described in Refs. [22,23]. We checked that this special integrator gives the smallest error (in the intersecting range of time steps) among six different second- and fourth-order integrators [12,26–28].

Conservation of the normalization N was checked numerically, relative errors (due to roundoff; we used double precision arithmetic throughout this paper) typically being of order 10^{-11}. Energy is not conserved exactly, and the relative error was of order 10^{-7} after an evolution time $t=500$ with an integration time step $\Delta t=0.0025$. The precise value depends, of course, on the parameters of the soliton and on x_0. We checked carefully that our results were independent of the time step and of the spatial discretization Δx.

In the following runs we used $\Delta t=0.01$, $\Delta x=\pi/16\approx0.2$, $a_0=\frac{1}{2}$, and $v_0=0.8$. So the initial soliton takes the form

$$\Psi(x,t=0)=\{2\cosh[\tfrac{1}{2}(x-50)]\}^{-1}e^{i0.8x}\ . \tag{8}$$

The kinetic energy of the soliton is, according to Eq. (5), $K=v_0^2/2=0.32$.

As we said, we are mostly interested in potential heights $V_0\approx K$, and in small slopes, $x_0\gg1$. But for completeness, we made also simulations in the entire region $0.28\le V_0\le0.38$, $0\le x_0\le25$. Our results for the transmission coefficients are shown in Fig. 1. Let us now discuss these results in detail.

(1) For $V_0\ge0.36$, i.e., far above the kinetic energy K, the transmission coefficients are both small and tend to zero for $x_0\to\infty$. But this convergence is not monotonic, as there is a maximum for $x_0\approx2-3$ that seems to be a nonlinear resonance effect. Also, T_N is systematically lower than T_E, which is easily understood.

(2) These data show a very slight shoulder at $5<x_0<10$. This shoulder gets more pronounced and is shifted towards larger values of x_0 when V_0 is decreased, but still stays larger than K. When V_0 reaches K, the shoulder is shifted to $x_0\approx12$ and is a dominating feature.

(3) As we decrease V_0 further, below K, this shoulder continues to become sharper and more pronounced. Indeed, it develops into a peak, and both transmission coefficients drop very steeply beyond this peak. After this drop, they seem to join a common curve independent of V_0, but they do not stay on this curve as we increase x_0 further. Indeed, we are now in a regime where classically the soliton could be fully transmitted, and T_E and T_N have to converge to 1 for $x_0\to\infty$. But we see that this limit is not reached smoothly. Instead, the transmission coefficients jump—instantaneously within our resolution—to values ≈1. The values of x_0 where these jumps happen seem to diverge when $V_0\to K$ from below.

(4) As V_0 is decreased further, we reach a value $V_{0,c}$ (numerically, $\approx0.3155\pm0.0005$) where the window of small transmission coefficients disappears. As $V_{0,c}$ is reached from above, the locations of the downward jump and of the upward jump both tend towards $x_{0,c}\approx14.7$. At this point, both jumps seem to be instrumentally

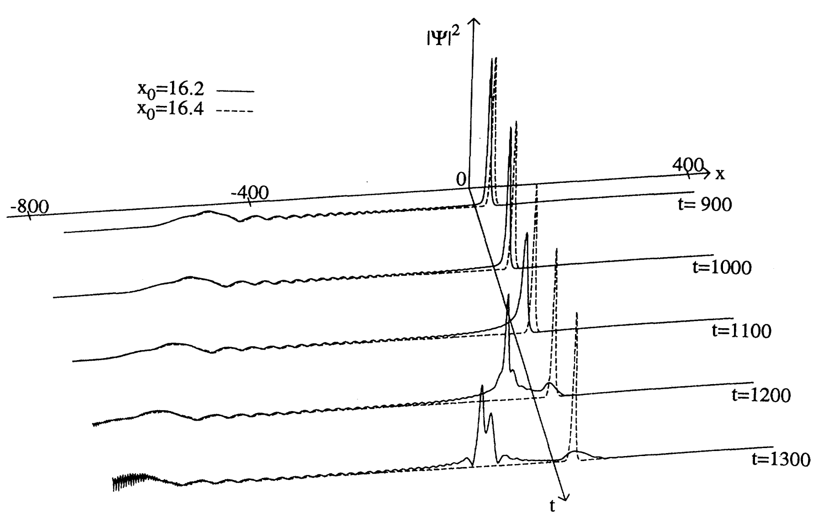

FIG. 2. Time evolution of $|\Psi|^2$ for two solitons with incident velocity $v_0=0.8$, which are scattered at a potential ramp with height $V_0=0.3165\approx0.989K_0$ and with $x_0=16.2$ (full line) and 16.4 (dashed line). The nonsolitary waves in the left-hand region ($x<-200$) are emitted when the soliton hits first the potential at $x=0$, $t\approx60$. The calculation was done on a lattice with 4096 sites, discretization width $\Delta x\approx0.2$, and integration step $\Delta t=0.01$.

sharp. For $V_0 < V_{0,c}$, no trace of this singular behavior is left, and the transmission coefficients rise monotonically toward their asymptotic value 1 as x_0 is increased.

(5) This monotonic rise is seen for $x_0 > 10$. For smaller values of x_0 we still see the maximum at $x_0 \approx 3$ that persisted throughout the above range, and that disappears only for $V_0 \lesssim 0.3$.

The unexpected and surprising behavior are the windows of small transmission coefficients seen for $V_{0,c} < V_0 < K$. This effect is not predicted classically (where we would have expected complete transmission), and is not clear *a priori* why the quantum theory should produce any structure that seems to be discontinuous to the naked eye.

To understand this, we first try to get some more insight by looking at the evolution of the wave function. In Fig. 2 we show $|\Psi|^2$ for $V_0 = 0.3165 \approx 0.989K$. In this plot we show both the effect of a ramp with $x_0 = 16.2$ (where the soliton is reflected; full line) and that of a ramp with $x_0 = 16.4$ (where it is transmitted; dashed line). The same two situations are compared in Fig. 3 where the local maxima of $|\Psi|^2$ are shown as functions of time. We see that in both situations the behavior is very similar for times < 800: when the soliton hits the potential, it is stopped to velocity near zero, and radiates nonsolitary waves back into region I where it comes from. This takes place during ≈ 100 time units. After this, the soliton nearly stays at rest, until it either moves slowly away from the interface ($x_0 = 16.4$) or falls back the slope ($x_0 = 16.2$) and is reflected.

A heuristic explanation of our effect—more precisely of the second jump, the first (downward) jump is less easy to understand—is now easily suggested. If there were no radiation (as is the case for $x_0 \to \infty$) the energy of the soliton would be conserved, and the threshold for transmission would be strictly at $V_0 = K$. But for finite x_0, the radiation implies that the soliton has lost energy when it reaches the upper end of the ramp, and it needs $K > V_0$ to be transmitted. Thus there is a range $K - \delta(x_0) < V_0 < K$ where the soliton is reflected though it would be transmitted classically. Since the soliton stays very long near the upper edge of the ramp for $V_0 \approx K - \delta(x_0)$, the dependence of the transmission coefficients on the amount of radiation (and thus also on x_0) is extremely steep. This explains very naturally the second (upward) jump of the transmission coefficients. It does not explain the first (downward) jump, for which we still have no good explanation.

To be more quantitative, let us consider $V_0 = 0.3190$. Here, the second jump (from nearly total reflection to nearly total transmission) occurs at $x_0 = 22.1 \equiv x_c$. At this slope, T_E jumps from 0.0093 to 0.9837, while T_N jumps from 0.0074 to 0.9797. The fact that the soliton is coming to a stop for $x_0 = x_c + \epsilon$ means that all its energy is potential energy, $E' = N'(V_0 - a'^2/6)$, and the energy difference goes into radiation. If we neglect the forward radiation (which seems to be indeed small according to Figs. 2 and 3), we have $N' = T_N$, $E' = T_E E_0$, and $a' = (T_N/2)^2$, and thus $T_E = T_N(V_0 - T_N^2/24)/E_0 = 0.9821$ for $x_0 = x_c + \epsilon$. Comparing this with the measured value 0.9837 we see good agreement.

This argument suggests that the observed effect survives if we replace the potential step by a barrier

$$V(x) = \begin{cases} 0\ , & x < 0 \\ xV_0/x_0\ , & 0 \le x < x_0 \\ V_0\ , & x_0 \le x < x_1 \\ (x - x_2)V_0/(x_1 - x_2)\ , & x_1 \le x < x_2 \\ 0\ , & x_2 \le x\ , \end{cases} \tag{9}$$

which goes back to zero for $x \to \infty$. We checked that this is indeed the case, provided $x_2 - x_1 \gg x_0 \gg 1$. In this case, the transmission coefficients are nearly the same as for the ramp with the same x_0 and V_0: i.e., the soliton overcomes a flat barrier if and only if it overcomes its ris-

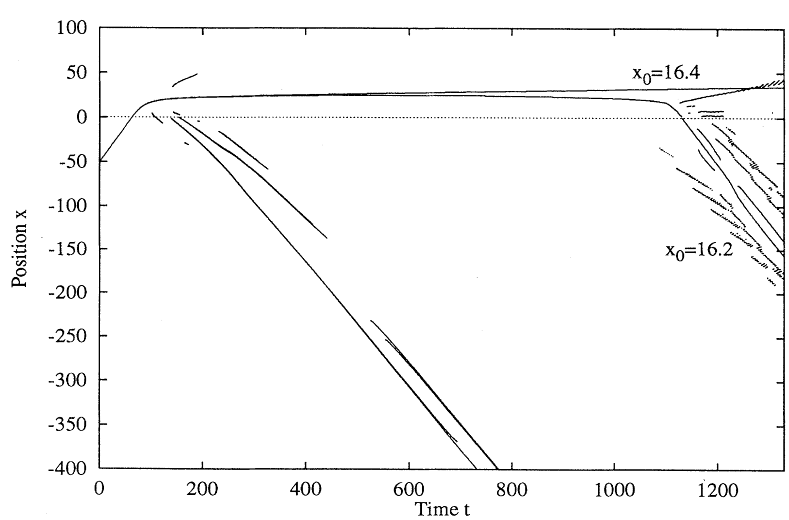

FIG. 3. Time evolution of local maxima of $|\Psi|^2$, where only the maxima $|\Psi|^2 > 1/3000$ are plotted. The parameters are the same as in Fig. 2.

ing part.

The above argument suggests also that a similar effect should be seen if the interface is not modeled by a linearly rising potential. For instance, we might consider a sigmoidal potential or a Gaussian barrier. In this case, the soliton still should radiate when hitting the region where the potential is varying (although maybe less than in the present case), and we expect a similar phenomenon. The same should be true if we describe the spatial inhomogeneity not by a spatially dependent $V(x)$ but by a spatial dependence of the coefficients in front of the kinetic or nonlinear terms of the NLSE. Also in these cases there should be radiation when the soliton encounters the inhomogeneity, such that its energy is lowered and it cannot penetrate a barrier that it otherwise would have just barely overcome.

Though we have not yet any definite application in mind, we believe that this effect an be of potential use for constructing switches in optical fibers or similar soliton-bearing devices.

We want to thank A. Torcini for reading carefully the manuscript. This work was partly supported by DFG within the Graduiertenkolleg "Feldtheoretische und numerische Methoden in der Elementarteilchen-und Statistischen Physik," and within SFB 237.

---

[1] H. Hasimoto and H. Ono, J. Phys. Soc. Jpn. **52**, 4129 (1983).
[2] G. L. Lamb, Jr., *Elements of Soliton Theory* (Wiley, Toronto, 1980).
[3] Yu. S. Kivshar *et al.*, Rev. Mod. Phys. **61**, 763 (1989).
[4] Yu. S. Kivshar *et al.*, Phys. Rev. A **41**, 1677 (1990).
[5] Yu. S. Kivshar and M. L. Quiroga-Teixeiro, Phys. Rev. A **48**, 4750 (1993).
[6] R. Jackiw, Rev. Mod. Phys. **49**, 681 (1977).
[7] J. P. Gordon, J. Opt. Soc. Am. B **9**, 91 (1992).
[8] M. Chbat *et al.*, J. Opt. Soc. Am. B **10**, 1386 (1993).
[9] D. Anderson *et al.*, J. Opt. Soc. Am. B **11**, 2380 (1994).
[10] M. A. Moura, J. Phys. A **27**, 7157 (1994).
[11] Yu. S. Kivshar *et al.*, Zh. Eksp. Teor. Fiz. **93**, 968 (1987) [Sov. Phys. JETP **66**, 545 (1987)].
[12] H. Yoshida, Phys. Lett. A **150**, 262 (1990).
[13] H. Yoshida, Cel. Mech. Dyn. Astron. **56**, 27 (1993).
[14] J. M. Sanz-Serna, Physica D **60**, 293 (1992).
[15] A. D. Bandrauk and Hai Shen, Chem. Phys. Lett. **176**, 428 (1991).
[16] K. Takahashi and K. Ikeda (unpublished).
[17] H. Frauenkron and P. Grassberger, Int. J. Mod. Phys. C **5**, 37 (1994).
[18] A. Rouhi and J. Wright, Comput. Phys. Commun. **85**, 18 (1995).
[19] D. Pathria and J. L. Morris, J. Comput. Phys. **87**, 108 (1990).
[20] J. A. C. Weideman and B. M. Herbst, SIAM J. Numer. Anal. **23**, 485 (1986).
[21] A.D. Bandrauk and Hai Shen, J. Phys. A **27**, 7147 (1994).
[22] R. I. McLachlan, Numer. Math. **66**, 465 (1994).
[23] H. Frauenkron and P. Grassberger, J. Phys. A **28**, 4987 (1995).
[24] P. G. Drazin and R. S. Johnson, *Solitons: An Introduction* (Cambridge University Press, New York, 1989).
[25] R. I. McLachlan and P. Atela, Nonlinearity **5**, 541 (1992).
[26] M. J. Ablowitz and C. Schober, Int. J. Mod. Phys. C **5**, 397 (1994).
[27] R. I. McLachlan, SIAM J. Sci. Comput. **16**, 151 (1995).
[28] L. Verlet, Phys. Rev. **159**, 98 (1967).