# Solitons and Bound States of the Time-Independent Schrödinger Equation

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A numerical calculation validates the correspondence between the soliton nonlinear asymptotic solutions of the time-dependent Korteweg–deVries equation and the bound states of the one-dimensional time-independent Schrödinger equation. Here the attractive potential of the Schrödinger equation is equal to the initial condition of the Korteweg–deVries equation. A situation is examined where an oscillatory state remains after solitons have emerged.

## I. INTRODUCTION

THE *soliton*, a nonlinear dispersive wave entity, has been introduced[1,2] to describe the dynamics of a class of wave interactions observed in solutions of the Korteweg-deVries (KdV) equation

$$u_t+\alpha uu_x+\delta^2u_{xxx}=0. \tag{1}$$

For a large class of nondissipative physical systems, Gardner and Su[3] and also Taniuti and Wei[4] have shown that the KdV equation describes the dynamics of small but finite perturbations about homogeneous equilibria. The simplification is obtained by applying uniform asymptotic methods to a system of coupled Eulerian-type mass and momentum conservation equations.

Earlier work applied asymptotic methods to specific physical situations and recovered the KdV equation: shallow water waves,[5] magnetohydrodynamic waves in a warm plasma,[6] ion-acoustic waves,[7] and acoustic waves in an anharmonic crystal.[8]

In Refs. 1 and 2 we demonstrated[9] numerically that solitons are remarkably stable—that is, when many solitons interact nonlinearly in a small spatial region, each emerges after a finite time with its identity preserved. Recently Lax[10] showed by rigorous analytical methods that two solitons are preserved through interaction, and it appears that his method of proof is valid in the general case of an arbitrary finite number of solitons. Berezin and Karpman[11] gave an heuristic method for predicting the number and speed of solitons that emerge from arbitrary initial conditions.

Miura[12] recently discovered a transformation (an inhomogeneous Ricatti equation) between solutions of the KdV equation and solutions of another equation obtained from (1) by replacing $\alpha uu_x$ by $\alpha u^2u_x$. Following this, Gardner, Greene, Kruskal, and Miura[13] (GGKM) *linearized* the problem and developed a rigorous method for treating the KdV equation and can determine the number and properties of emerging solitons. In this paper a numerical algorithm for solving the KdV equation with periodic boundary conditions or with boundary conditions approximating the infinite interval is given. In the latter case, when the initial condition is chosen to decompose into only two solitons, good agreement between numerical and analytical solutions is obtained. Furthermore, an initial condition is studied that leads to one soliton and an oscillatory state, and properties of the latter state are given.

## II. ANALYTICAL PROPERTIES OF A $\mathrm{sech}^2(x)$ INITIAL CONDITION

In order to compare results with those of GGKM we rewrite the KdV equation as

$$u_t-6uu_x+u_{xxx}=0. \tag{2}$$

For an initial condition of given spatial extent or width, the *single* parameter that characterizes the solutions is the amplitude. The larger the magnitude of the initial amplitude, the more nonlinear and less dispersive is the character of the solution. Unlike the 1965 paper[1] where $\alpha>0$, solitons in this paper will have *negative* amplitudes, but will still travel to the right because the signs before $u_t$ and $u_{xxx}$ are identical.

GGKM showed that if $u(x,t)$ changes with time, according to the KdV equation, then the eigenvalues $\lambda_n$,

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[1] N. J. Zabusky and M. D. Kruskal, Phys. Rev. Letters **15**, 240 (1965).

[2] N. J. Zabusky, in *Proceedings of the Symposium on Nonlinear Partial Differential Equations*, edited by W. Ames (Academic Press Inc., New York, 1967).

[3] C. S. Gardner and C. H. Su, Annual Report, Princeton University Plasma Physics Laboratory, Matt-Q-24, 1967, p. 329 (unpublished).

[4] T. Taniuti and C.-C. Wei, Nagoya University, Japan, Physics Department Report, 1967 (unpublished).

[5] D. J. Korteweg and G. deVries, Phil. Mag. **39**, 422 (1895).

[6] C. S. Gardner and G. K. Morikawa, Comm. Pure Appl. Math. **18**, 35 (1965); also, New York University Report NYO 9082, 1960 (unpublished).

[7] H. Washimi and T. Taniuti, Phys. Rev. Letters **17**, 966 (1966).

[8] N. J. Zabusky, in *Proceedings of the Conference on Mathematical Models in the Physical Sciences*, edited by Stefan Drobot (Prentice Hall, Inc., Englewood Cliffs, N. J., 1963), p. 99.

[9] It is known and easily demonstrated that if $u(x,t)$ is periodic or localized in the region $(L_1,L_2)$

$$M=\int_{L_1}^{L_2} udx \quad\text{and}\quad E=\int_{L_1}^{L_2}\tfrac{1}{2}u^2dx$$

are time-invariant quantities. (In fact, we have shown that the KdV equation has an infinity of independent invariant quantities). By "demonstrated" we mean that when solitons interacted, not only were their amplitudes preserved to high accuracy but also $M$ and $E$ were constant to the accuracy of the numerical calculation.

[10] P. D. Lax (private communication).

[11] Yu. A. Berezin and V. I. Karpman, Zh. Eksperim. i Teor. Fiz. **51**, 1557 (1966) [English transl.: Soviet Phys.—JETP **24**, 1049 (1967)].

[12] R. Miura, J. Math. Phys. (to be published).

[13] C. S. Gardner, J. M. Greene, M. D. Kruskal, and R. M. Miura, Phys. Rev. Letters **19**, 1095 (1967).

($n=0, 1, 2, 3, \cdots, N-1$) defined by the one-dimensional time-independent Schrödinger equation (3) are time invariant:

$$\psi_{xx}^{(n)}-[u(x,t)-\lambda_n]\psi^{(n)}=0. \tag{3}$$

[The time $t$ in (3) is a parameter and does not correspond to the usual time in Schrödinger's equation.] Thus, the eigenvalues of the discrete spectrum $\lambda_n<0$ (the bound-state eigenvalues) are preserved and are associated with the amplitudes of the solitons that emerge from an arbitrary, smooth, square-integrable initial state $u(x,0)$. In particular, the solitons will have

$$\text{amplitudes,}\quad A_n=2\lambda_n;$$

and

$$\text{speeds,}\quad c_n=\tfrac{1}{3}\alpha A_n=-4\lambda_n. \tag{4}$$

Some consequences of this are:

(1) If $\int_{-\infty}^{+\infty}u(x,0)dx<0$ (corresponding to a one-dimensional attractive potential) there will always be at least one bound state and hence $u(x,t)$ for $t$ large has at least one soliton.

(2) The strong potential or large amplitude initial condition limit is characterized by a parameter proportional to $u_0l^2$, where $u_0$ and $l$ are the depth and width of the well, respectively. In any standard text in quantum mechanics one finds that if $u_0l^2$ is large (1) the number of bound states or solitons is proportional to $l(u_0)^{1/2}$; and (2) a plot of $|\lambda_n|$ versus $n$ for the largest eigenvalues gives a straight line. Thus at a given time $\tau\gg0$, the minima of the strongest solitons will also lie on a straight line, a fact observed in previous numerical calculations with *periodic* boundary conditions (Ref. 1, Fig. 1).

(3) The KdV equation conserves total momentum and energy. Thus the momentum and energy that finally do not reside in solitons will reside in another state—the oscillatory "tail" that spreads to the left. It has been observed in numerical calculations and is related to the continuous spectrum of (3).

To compare with GGKM and to validate our ideas, let us solve (2) with the specific initial condition

$$u(x,0)=-p(p+1)\operatorname{sech}^2x, \tag{5}$$

where $p>0$. The bound-state eigenvalues in ascending order are given by[14]

$$\lambda_n=-(p-n)^2=-(\epsilon-1+N-n)^2, \qquad (n=0, 1, \cdots, N-1) \tag{6}$$

where $N$ is the total number of bound states, i.e., it is the largest *integer* satisfying the inequality $N\le p+1$, and $\epsilon$ is defined in the range $0\le\epsilon<1$ by

$$\epsilon=1+p-N. \tag{7}$$

If $p$ is an integer, then $\epsilon=0$ and the initial state of the KdV equation will decompose only into solitons. If $p_1$ and $p_2$ ($p_1>p_2$) are nonintegers, then the $N_2$ solitons of smallest magnitude that emerge from both initial conditions are identical in size, namely, they have the amplitudes $-2\epsilon^2, -2(\epsilon+1)^2, -2(\epsilon+2)^2, \cdots, -2(\epsilon+N_2-1)^2$.

Table I gives the total momentum, $\int_{-\infty}^{+\infty}udx$, and total energy, $\frac{1}{2}\int_{-\infty}^{+\infty}u^2dx$, corresponding to the initial condition (5) and also the component in the oscillatory tail (that is, after the momentum and energy in the solitons has been subtracted from column 1).

Note that the momentum of the tail is positive and the momentum and energy are independent of $N$. That is, for given $\epsilon$ and *different* $N$ the tail solutions are probably identical.

Karpman[15] (see notation in Ref. 15) gives the distribution function of soliton amplitude for a large amplitude initial condition defined by $u(x,0)=u_0\operatorname{sech}^2(x/l)$. The distribution function agrees with the exact result obtained from (6) with $A=2\lambda$, namely,

$$f(A)=|dA/dn|^{-1}=|4(p-n)|^{-1}=(8|A|)^{-1/2}.$$

If we define $\eta=|A|/u_0$ [where $|u_0|=p(p+1)$], then $f(\eta)=(u_0/8\eta)^{1/2}$, which is Karpman's equation (8) when $\beta=l=1$ and $(u_0/6)\to u_0$ (since we take $|\alpha|=6$ and he uses $\alpha=1$ and $\delta^2=\beta$).

## III. NUMERICAL ALGORITHM AND ANALYTICAL/NUMERICAL COMPARISONS

### A. Numerical Integration Algorithm

To solve (1), we used the four point, left-sweeping, two-time-level numerical algorithm[16]

$$\begin{aligned}0=(\delta^2/h^3)[&s(i+2, j+1)-3s(i+1, j)\\&+3s(i, j+1)-s(i-1, j)]\\&+(\alpha/8h)[s(i+2, j+1)+s(i-1, j)]\\&\times[s(i+2, j+1)+s(i+1, j)\\&\qquad-s(i, j+1)-s(i-1, j)],\end{aligned} \tag{8}$$

where

$$s(i,j)\to u(x/h, t/k), \tag{9}$$

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[14] See, for example, L. Landau and E. Lifschitz, *Quantum Mechanics, Nonrelativistic Theory* (Pergamon Press, Inc., New York, 1958), p. 69.

[15] V. I. Karpman, Phys. Letters **25**, 708 (1967). In this paper, use is made of the Korteweg-deVries conservation laws (Ref. 2) to obtain the *asymptotic* distribution of soliton amplitudes $f(\eta)$ and total number of solitons $N$ emerging from a given large amplitude initial condition. Here $\eta$=soliton amplitude/$u_0$. Karpman writes his KdV equation as $u_t+uu_x+\beta u_{xxx}=0$ and his initial condition as $u(x,0)=u_0\operatorname{sech}^2(x/l)$ and obtains

$$\text{(Eq. 8)}\quad f(\eta)=l(u_0/48\beta\eta)^{1/2},$$

and

$$\text{(Eq. 9)}\quad N=l(u_0/6\beta)^{1/2}.$$

To compare his results with ours, set $l=\beta=1$ and set his $u_0/6$ to our $u_0$.

[16] The algorithm actually used was obtained by rearranging (8) and setting $\delta^2=1$, $\alpha=-6$, namely,

$$s(i, j+1)=s(i+1, j)-[s(i+2, j+1)-s(i-1, j)][(1+\bar{s})/(3-\bar{s})],$$

where

$$\bar{s}=-(3h^5/4)[s(i+2, j+1)+s(i-1, j)],$$

and

$$s(i,j)=(1/4k)u(x/h, t/k).$$

Both runs described in this paper were made with $h=1/25$.

TABLE I. Momentum and energy for the initial condition $u(x,0)=-p(p+1)\,\mathrm{sech}^2(x)$.

| | Total | Tail |
|---|---|---|
| Momentum | $-2p(p+1)$ | $+2\epsilon(1-\epsilon)$ |
| Energy | $+(\frac{2}{3})p^2(p+1)^2$ | $+(\frac{2}{3})\epsilon^2(1-\epsilon)^2$ |

and $h$ and $k$ are the spatial and temporal intervals between lattice positions that must satisfy

$$k=h^3/4\delta^2. \tag{10}$$

Condition (10) is obtained if one makes a Taylor-series expansion of (8), namely,

$$u_t+\alpha uu_x+\delta^2 u_{xxx}=-(h^2/8)\{3u_{txx}+\delta^2 u_{xxxxx}+\alpha[(7/3)uu_{xxx}+9u_x u_{xx}]\}+O(h^3). \tag{11}$$

The right side of (11) contains lowest-order continuum limit terms of the discretization error. Locally, these errors are of order $(h^2/\Delta^2)$ and $\alpha A(h^2/\Delta^2)$ where $A$ and $\Delta$ are the amplitude and half-width of a soliton $[\Delta=\delta(12/\alpha A)^{1/2}]$. Thus, only in the neighborhood of the largest solitons, namely, the ones having the smallest half-width $\Delta$, will we have a sizeable discretization error. One can show that the linear operator given in the first bracket of (8) is marginally stable. With properly chosen $h$ and $k$ our computations were never unstable.

The two right boundary conditions are

$$u(x_R,t)=u_x(x_R,t)=0, \tag{12}$$

where $x_R=x_R(t)$ is translated so as to keep the leading minimum of $u$ (the smallest emerging soliton) a fixed, large distance from the right boundary. The left boundary condition is evaluated at a fixed location $x_L$

$$u(x_L,t)=u(x_L,0)=-p(p+1)\,\mathrm{sech}^2 x_L. \tag{13}$$

Note that $u(x_L,t)$ is very small since $x_L\leq -12.5$.

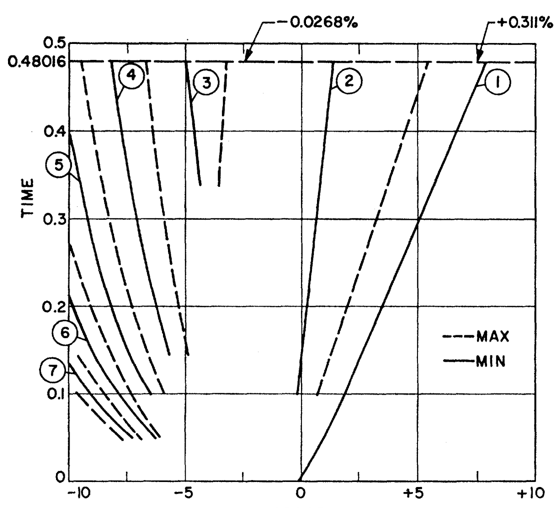


FIG. 1. Space-time diagram for the trajectories of the minima of $u(x,t)\,(p=2.0)$, Eq. (2).

These boundary conditions approximate the infinite interval for short times. The left boundary condition is the poorer approximation, since the linear terms of the KdV equation (2) cause perturbations $\exp i(\omega t-\kappa x)$ to propagate to the left with a group velocity $d\omega/d\kappa=-3\kappa^2$. To represent $u(x,t)$ accurately in the box $0\leq t\leq N_c k$, $x_L\leq x\leq x_R$, one should have a left boundary condition $u(\tilde{x}_L,t)=0$ where $\tilde{x}_L$ translates to the right and begins at $\tilde{x}_L=x_L-N_c h$ when $t=0$.

### B. Analytical/Numerical Comparisons

Two runs were made. For $p=2.0$, an exact solution has been obtained and we can compare and validate the algorithm; for $p=0.8$ only some properties of the exact solution are known and we can compare with these and predict other properties.

In Fig. 1 we give the space-time diagram for the loci of minima of the numerical solution of (2) with $p=2.0$. For this case, analysis tells us that only two solitons will emerge, i.e., the oscillatory state will have zero amplitude. GGKM have found the exact solution for this case:

$$u_E(x,t)=-12\left\{\frac{3+4\cosh(2x-8t)+\cosh(4x-64t)}{[3\cosh(x-28t)+\cosh(3x-36t)]^2}\right\}, \tag{14}$$

and in Table II we compare the numerical solution with the exact solutions and find that they are in very good agreement. The minima seen in Fig. 1 behind the two

TABLE II. Comparison of the numerical and exact solutions of the KdV equation (2) with $p=2.0$.

| | | First minimum | | Second minimum | |
|---|---|---|---|---|---|
| | $t$ | Amplitude | Location | Amplitude | Location |
| $u$(numerical) | 0.48016 | −7.978 | 7.9563 | −1.995 | 1.3634 |
| $u$(exact) | 0.48016 | −8.000 | 7.9572 | −2.000 | 1.3713 |
| $u$(exact) | ∞ | −8.000 | ··· | −2.000 | ··· |

leading minima arise because of truncation errors and round-off errors (that prevent any numerical computation from interpreting $p=2.0$ to more than eight significant figures). The boundary conditions (12) and (13) that approximate the semi-infinite interval may also contribute to these errors. These minima are in fact very small, e.g., at $t=0.48016$, $x=-2.483$, then

$$(100\%)(u_{\mathrm{Num}}-u_E)/|\min u(x,0)|=-0.027\%.$$

Alternatively, at $t=0.48016$ the energy associated with the oscillatory tail (in the range $-10\leq x\leq -2.76$) is $(6.5\times 10^{-6})\%$ of the total energy. The maximum difference between the numerical and exact solutions, [Eq. (14)] occurs at $x=7.506$ and is $0.311\%$.

For $p=0.8$, Table III compares the analytical predictions with numerical computations, and Fig. 2 shows

TABLE III. Comparison of analytical and numerical results for $u(x,0)=-(0.8)(1.8)\,\mathrm{sech}^2x$. [Entries are $I_n=\sum_{i=i_l}^{i_u}(1/n)u^n(ih,t)$ ($n=1$ for momentum, 2 for energy). Here $i=11$, corresponding to $x=ih=11/25=0.44$, is the location of the first zero crossing of $u(x,t)$ behind the emerging soliton.]

| | Time | Soliton amplitude | Soliton momentum | Soliton energy | Tail momentum | Tail energy |
|---|---|---|---|---|---|---|
| Analytical | $\infty$ | $-1.2800$ | $-3.200$ | $-1.3653$ | $+0.3200$ | $-0.01707$ |
| Numerical | 1.5321 | $-1.2838$ | $-3.155$[a] | $-1.3648$[a] | $+0.7145$[b] | $-0.01633$[b] |

[a] Soliton: $i_l=11$, $i_u=995$. [b] Tail: $i_l=-700$, $i_u=11$.

properties of the solution in the time interval $0\leq t\leq 1.5321$.

The theory indicates that for $p=0.8$ one soliton of amplitude $-1.280$ will emerge and leave behind an oscillatory state. The lower part of Fig. 2 is a space-time diagram of the trajectories of the minima of $u(x,t)$. At $t=0$ we see the single minimum at $x=0$, and at $t=0+$ we see an increasing density of minima as one moves to the left of $x=0$ (not all have been plotted). As $t$ increases, the smallest minimum moves off to the right and becomes our soliton. At $t=1.5321$ the minimum has translated to 3.780 and its value is $-1.2838$. The oscillatory tail has minima whose separation distance increases in time, and at a given time the separation distance decreases as one moves to the left. This is evident in the upper part of the figure where $u(x,1.5321)$ has been drawn on an expanded ordinate scale.

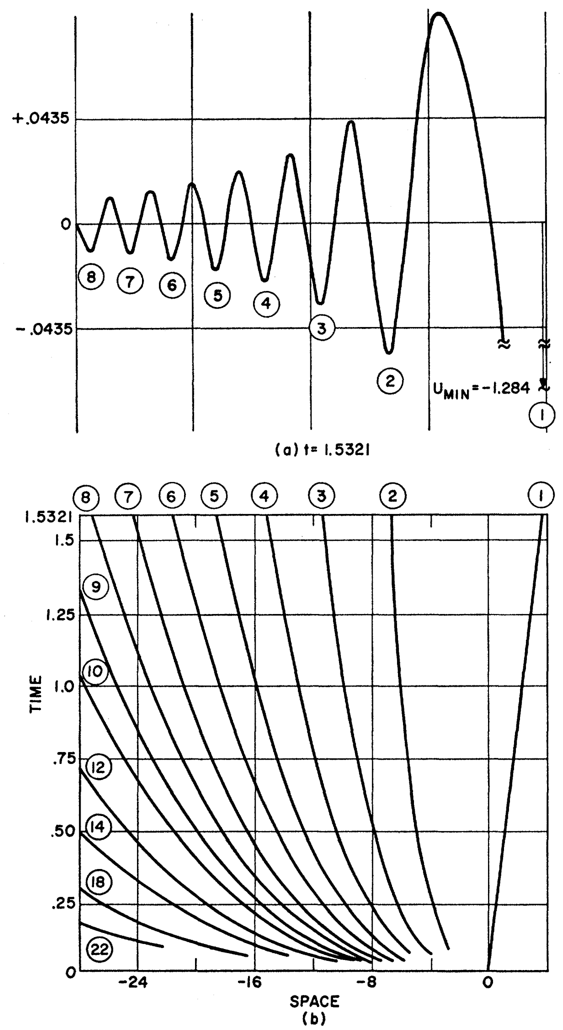


FIG. 2. (a) The waveform $u(x,7.660)$ exhibiting the amplitude of the soliton and the oscillatory state to the left (for $p=0.8$), Eq. (2). (b) Space-time diagram for the trajectories of the minima of $u(x,t)$ ($p=0.8$), Eq. (2).

In this run total energy decreased by 0.093% and total momentum (a negative quantity) decreased by 0.184%. The above data show that the observed soliton differs from the $t=\infty$ well-separated soliton by 0.30% in amplitude and 0.037% in energy. The tail energies differ by 4.54%. The apparently large error in tail momentum (Table III) is due to the fact that we are summing positive and negative numbers of comparable and small magnitude. Also the location, $i=11$, for the end of the soliton and beginning of the tail is arbitrary. Had we used a value of $i>11$ then we would have increased the tail energy and decreased the tail momentum, thereby obtaining better agreement with analytical results.

Note that at small $t$ and $x\gtrsim x_L$, the wavelength of the oscillations can become comparable to the mesh size $h$ and give large local discretization errors. These errors are very small relative to the initial condition amplitudes; since small perturbations propagate to the left, the "rough" structure disappears when $t>0.1$ and in its place arises a smooth oscillation of increasing wavelength, as shown in Fig. 2. For solutions of high accuracy numerical analysts should consider the long-range effect of these localized discretization errors.

The oscillatory tail may eventually be described analytically by solutions of the Gel'fand-Levitan equation, as alluded to in the work GGKM. A "reasonable" asymptotic formula for this state is

$$u(x,t)=F(x,t)\cos[\beta(x_0-x)^N/t^n+\varphi]\,, \tag{15}$$

where $F(x,t)$ is a slowly varying function of $x$ and $t$ that decreases monotonically as $x\to-\infty$. In Table IV we give three sets of the parameters $N$, $n$, and $\beta$, obtained by curve-fitting the numerical data at two different times and at four adjacent maxima and minima of $u$. For example, in row 1 we obtain $N$, $\beta/t^n$, $x_0$, and $\varphi$ at $t=0.1393$ by using minima 6 and 7 and the maxima to the left of these. Using the value of the location of

TABLE IV. Parameters for the asymptotic properties of the oscillatory state obtained by curve-fitting [$p=0.8$, Eq. (2)].

| $t$ | Near minima | $N$ | $n$ | $\beta$ |
|---|---|---|---|---|
| 0.1393 | 6,7 | 1.41 | 0.56 | 0.59 |
| 0.1393 | 12,13 | 1.41 | 0.54 | 0.58 |
| 1.5321 | 6,7 | 1.69 | 0.39 | 0.17 |

minimum 6 at two nearby times (see Fig. 2) we are able to calculate $\beta$ and $n$.

## IV. CONCLUSIONS

The theoretical work of Gardner, Greene, Kruskal, and Miura rigorously relates solutions of the Korteweg-deVries nonlinear partial differential equation to the Gel'fand-Levitan linear integral equation. They show that bound states of a one-dimensional potential well correspond to the soliton solutions of the KdV equation with the potential well used as an initial condition. Using these facts, we have validated a numerical integration algorithm for the KdV equation and have also determined properties of the oscillatory state which remain when the solitons propagate away. This validated algorithm can also be used for a situation having periodic boundary conditions, a case where no solutions have as yet been obtained.

Galvin and others[17] have observed soliton interactions among "secondary" water waves produced in a long tank by a sinusoidally moving piston. We intend to apply the numerical algorithm to establish in detail the physical regions where solutions of the KdV equation describe interactions among surface water waves.

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I wish to acknowledge helpful conversations with C. Gardner, J. Greene, M. Kruskal, R. Miura, and G. S. Deem. C. Gardner contributed to the derivation of the values given in Table I. Mrs. Katherine Goldman assisted with the numerical computations.

[17] C. J. Calvin, Jr., Coastal Engineering Research Center Report 1967 (unpublished).